



wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 07:58 PM BST

PDB ID : 4V97
Title : Crystal structure of the bacterial ribosome ram mutation G299A.
Authors : Fagan, C.E.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2012-04-06
Resolution : 3.52 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

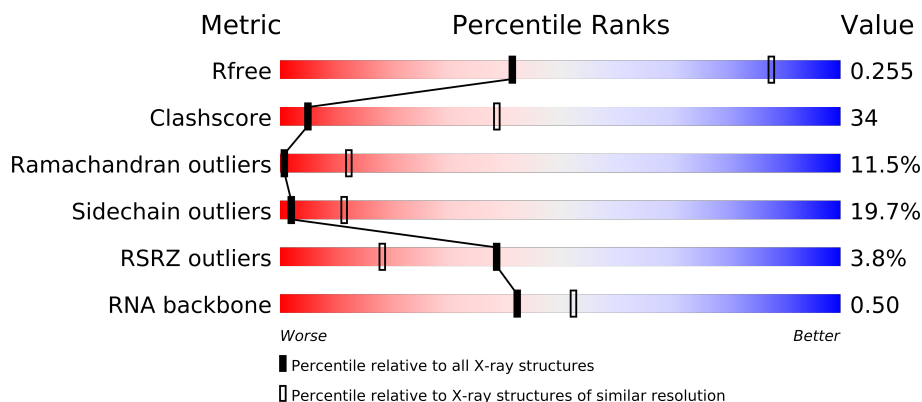
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable23397
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23397

1 Overall quality at a glance

The reported resolution of this entry is 3.52 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1256 (3.74-3.30)
Clashscore	79885	1020 (3.68-3.36)
Ramachandran outliers	78287	1082 (3.70-3.34)
Sidechain outliers	78261	1082 (3.70-3.34)
RSRZ outliers	66119	1256 (3.74-3.30)
RNA backbone	1838	1008 (4.26-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1522	
1	CA	1522	
2	AB	256	
2	CB	256	
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	

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Mol	Chain	Length	Quality of chain
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	77	
22	CV	77	
23	AW	76	
23	AY	76	
23	CW	76	
23	CY	76	
24	AX	24	
24	CX	24	
25	BA	2915	
25	DA	2915	
26	BB	122	
26	DB	122	

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Mol	Chain	Length	Quality of chain
27	BC	229	
27	DC	229	
28	BD	276	
28	DD	276	
29	BE	206	
29	DE	206	
30	BF	210	
30	DF	210	
31	BG	182	
31	DG	182	
32	BH	180	
32	DH	180	
33	BI	148	
33	DI	148	
34	BN	140	
34	DN	140	
35	BO	122	
35	DO	122	
36	BP	150	
36	DP	150	
37	BQ	141	
37	DQ	141	
38	BR	118	
38	DR	118	
39	BS	112	
39	DS	112	
40	BT	146	
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	

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Mol	Chain	Length	Quality of chain
48	B1	98	
48	D1	98	
49	B2	72	
49	D2	72	
50	B3	60	
50	D3	60	
51	B4	71	
51	D4	71	
52	B5	60	
52	D5	60	
53	B6	54	
53	D6	54	
54	B7	49	
54	D7	49	
55	B8	65	
55	D8	65	
56	B9	37	
56	D9	37	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 293977 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32328	14390	5992	10443	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32328	14390	5992	10443	1503			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	299	A	G	ENGINEERED MUTATION	GB AP008226.1
CA	299	A	G	ENGINEERED MUTATION	GB AP008226.1

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1010	639	197	174			
9	CI	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called P-SITE tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	CV	77	Total	C	N	O	P	0	0	0
			1643	732	297	537	77			

- Molecule 23 is a RNA chain called E-SITE TRNA PHE OR A-SITE tRNA Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
23	AY	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
23	CW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
23	CY	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	12	Total	C	N	O	P	0	0	0
			255	115	46	82	12			
24	CX	10	Total	C	N	O	P	0	0	0
			210	96	39	66	9			

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2810	Total 60527	C 26937	N 11326	O 19455	P 2809	0	0	0
25	DA	2824	Total 60827	C 27071	N 11381	O 19552	P 2823	0	0	0

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	119	Total 2551	C 1136	N 471	O 826	P 118	0	0	0
26	DB	119	Total 2551	C 1136	N 471	O 826	P 118	0	0	0

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	BC	191	Total 1142	C 691	N 221	O 230	0	0	1
27	DC	191	Total 1142	C 691	N 221	O 230	0	0	1

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	272	Total 2105	C 1329	N 417	O 356	S 3	0	0	1
28	DD	272	Total 2105	C 1329	N 417	O 356	S 3	0	0	1

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BE	205	Total 1564	C 988	N 300	O 270	S 6	0	0	1
29	DE	205	Total 1564	C 988	N 300	O 270	S 6	0	0	1

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BF	208	Total 1624	C 1035	N 304	O 282	S 3	0	0	1

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	DF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
31	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
32	DH	168	Total	C	N	O	S	0	0	0
			1290	820	240	229	1			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
33	DI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
34	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
35	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
36	DP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
37	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BR	117	Total	C	N	O		0	0	0
			960	599	202	159				
38	DR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BS	99	Total	C	N	O		0	0	1
			771	486	155	130				
39	DS	111	Total	C	N	O		0	0	0
			882	556	176	150				

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
40	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
41	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
42	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
43	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BX	93	Total	C	N	O		0	0	1
			726	471	132	123				
44	DX	93	Total	C	N	O		0	0	1
			726	471	132	123				

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
45	DY	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
47	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
48	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
49	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
50	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			
51	D4	40	Total	C	N	O	S	0	0	1
			298	189	50	54	5			

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
52	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			
53	D6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
54	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
55	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
56	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

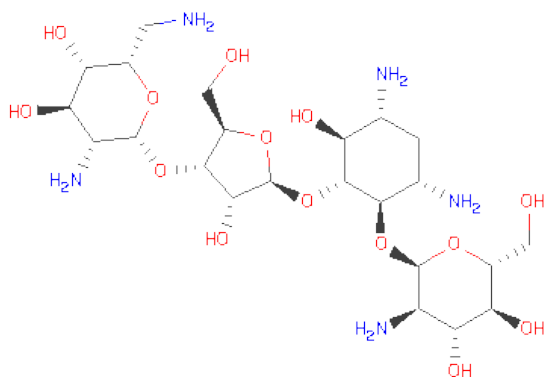
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	BA	323	Total Mg 323 323	0	0
57	CA	141	Total Mg 141 141	0	0
57	DQ	1	Total Mg 1 1	0	0
57	DF	1	Total Mg 1 1	0	0
57	CV	5	Total Mg 5 5	0	0
57	D2	1	Total Mg 1 1	0	0
57	BE	3	Total Mg 3 3	0	0
57	DU	3	Total Mg 3 3	0	0
57	BP	1	Total Mg 1 1	0	0
57	AX	1	Total Mg 1 1	0	0
57	CY	1	Total Mg 1 1	0	0
57	DD	3	Total Mg 3 3	0	0
57	B5	1	Total Mg 1 1	0	0
57	BB	5	Total Mg 5 5	0	0
57	AE	1	Total Mg 1 1	0	0
57	BF	1	Total Mg 1 1	0	0
57	AV	5	Total Mg 5 5	0	0
57	D8	1	Total Mg 1 1	0	0
57	AA	110	Total Mg 110 110	0	0
57	CX	1	Total Mg 1 1	0	0
57	BU	1	Total Mg 1 1	0	0
57	BN	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	D0	2	Total 2	Mg 2	0	0
57	DE	2	Total 2	Mg 2	0	0
57	DX	1	Total 1	Mg 1	0	0
57	DA	397	Total 397	Mg 397	0	0
57	DW	1	Total 1	Mg 1	0	0
57	B7	1	Total 1	Mg 1	0	0
57	BO	1	Total 1	Mg 1	0	0
57	D1	2	Total 2	Mg 2	0	0
57	DP	3	Total 3	Mg 3	0	0
57	CW	1	Total 1	Mg 1	0	0
57	D5	2	Total 2	Mg 2	0	0
57	BD	2	Total 2	Mg 2	0	0
57	CE	2	Total 2	Mg 2	0	0
57	DB	5	Total 5	Mg 5	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	AA	1	Total	C	N	O	0	0
			42	23	5	14		
58	CA	1	Total	C	N	O	0	0
			42	23	5	14		

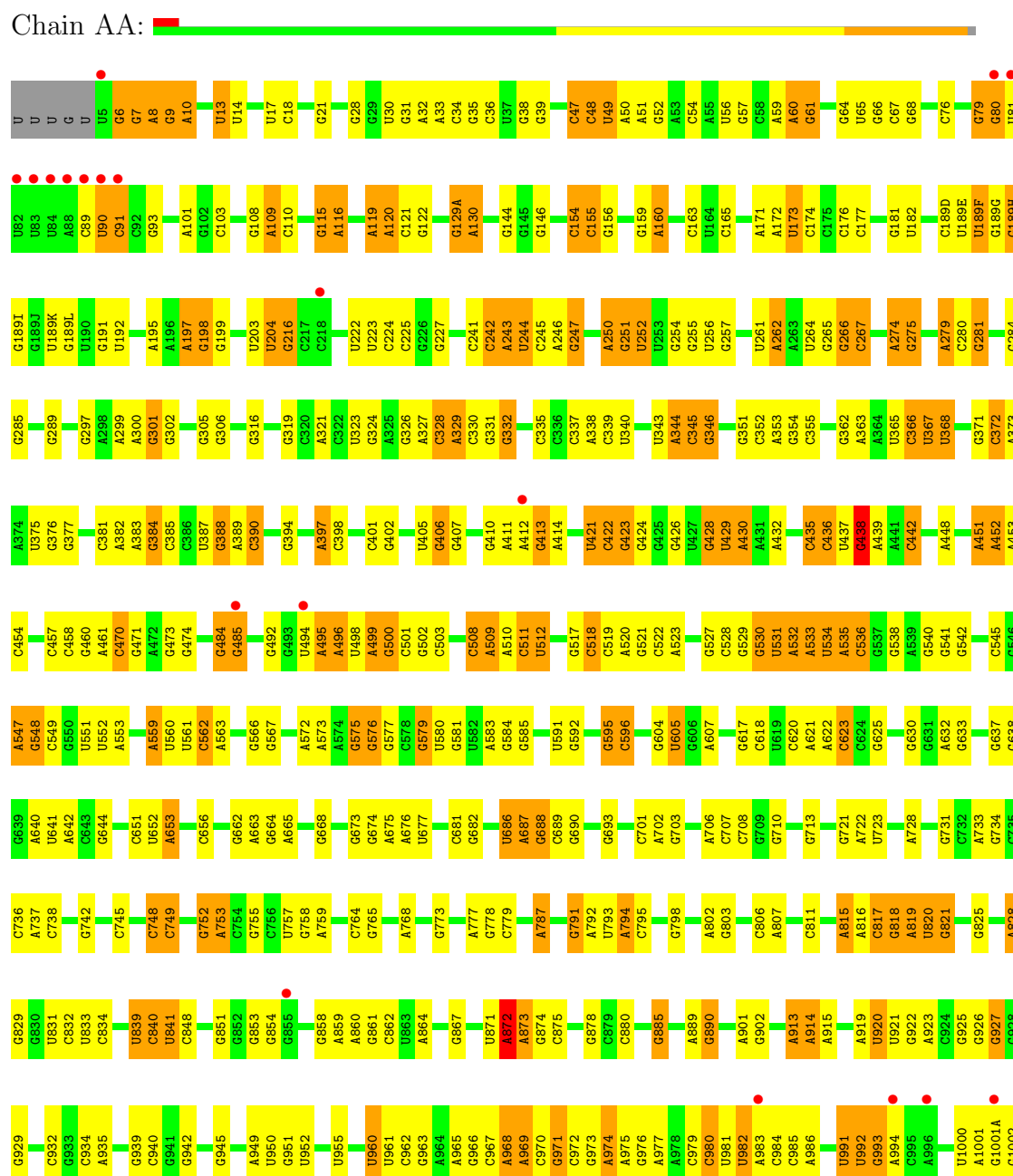
- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

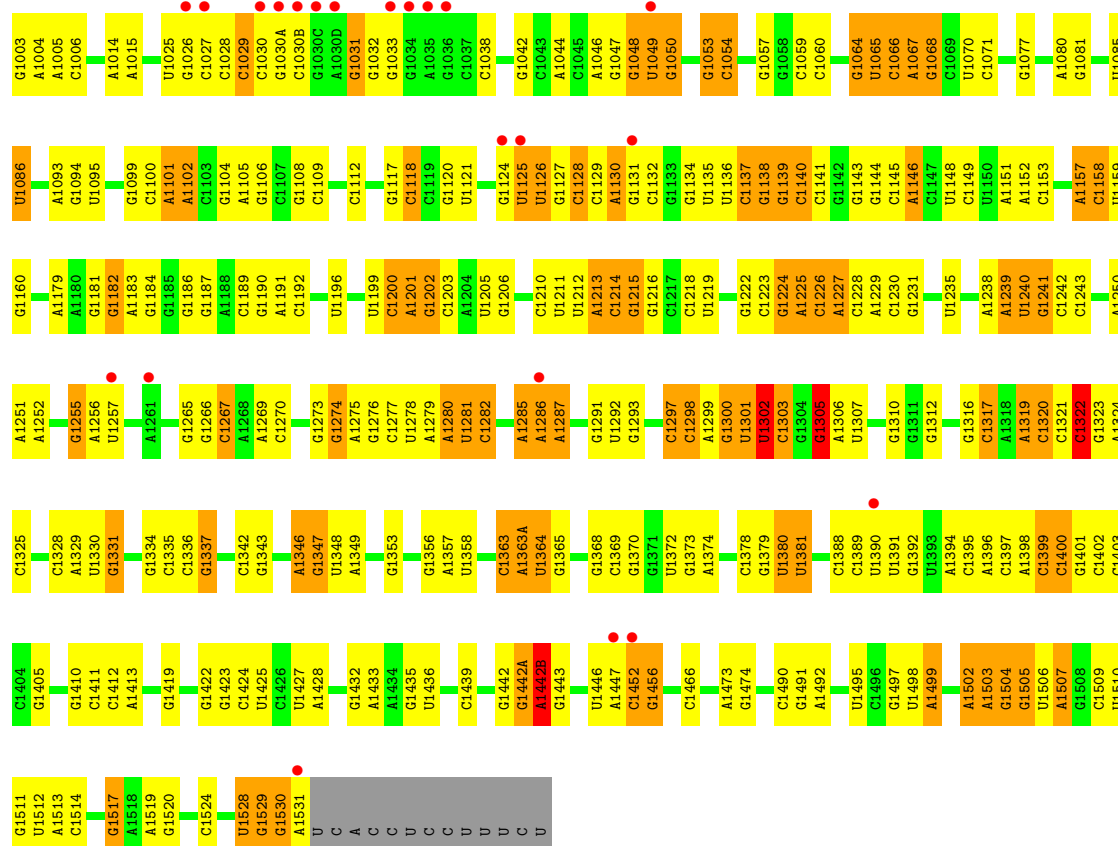
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	CN	1	Total	Zn	0	0
			1	1		
59	AD	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

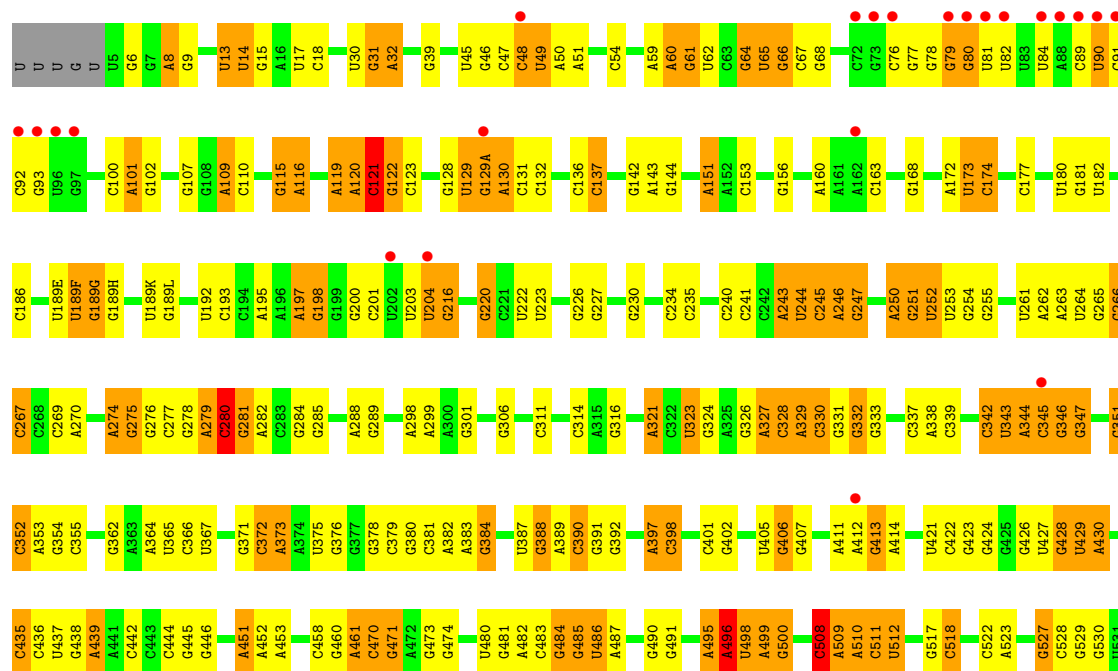
• Molecule 1: 16S rRNA

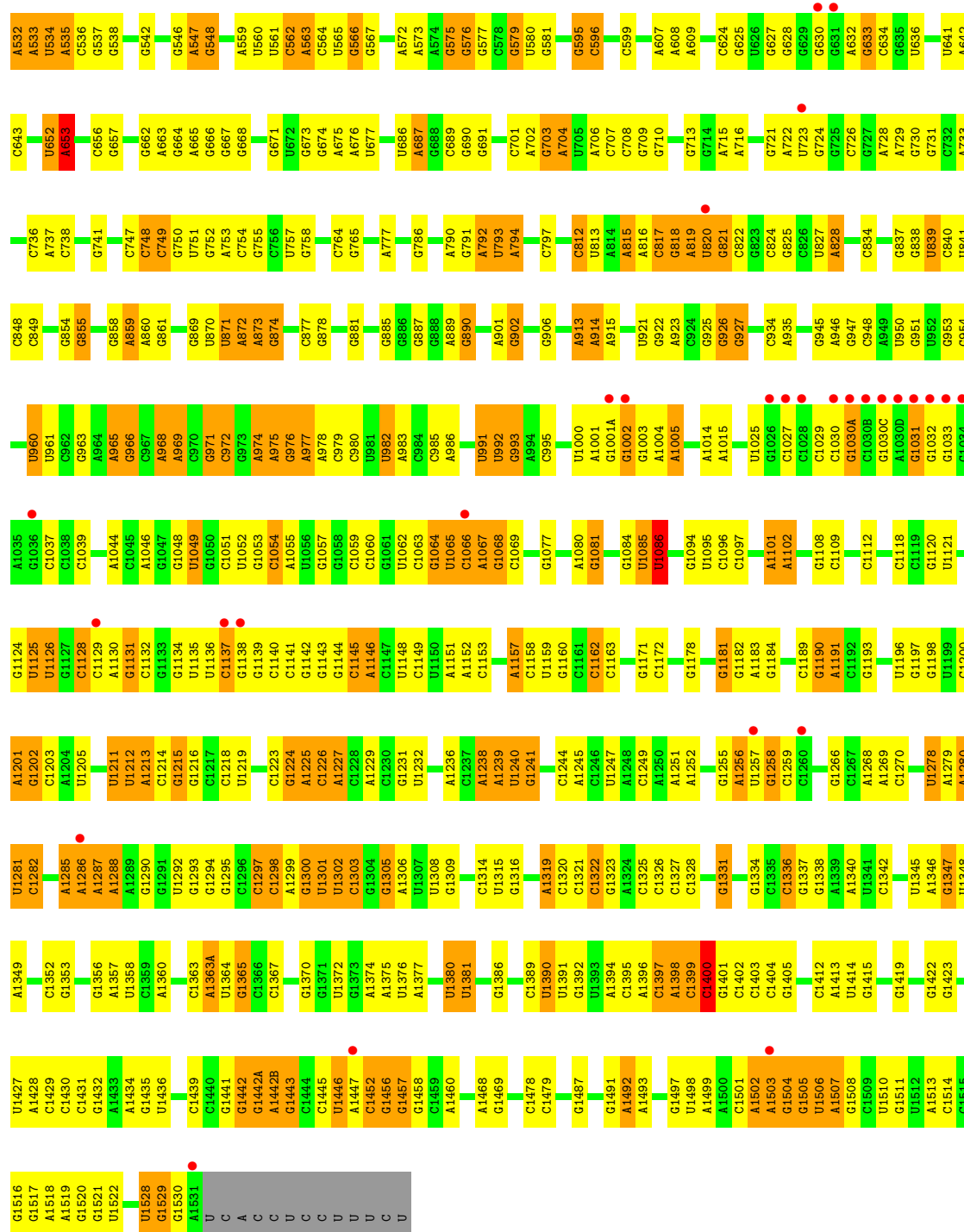




• Molecule 1: 16S rRNA

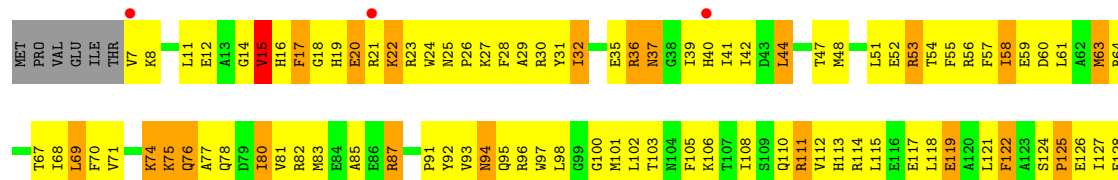
Chain CA:

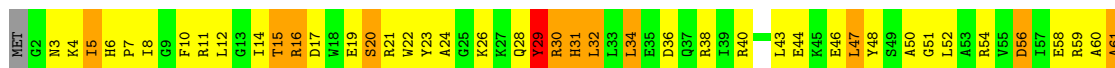


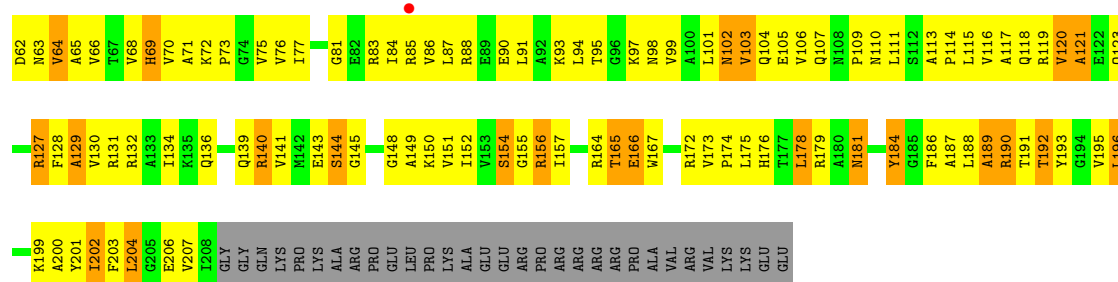


• Molecule 2: 30S ribosomal protein S2

Chain AB:

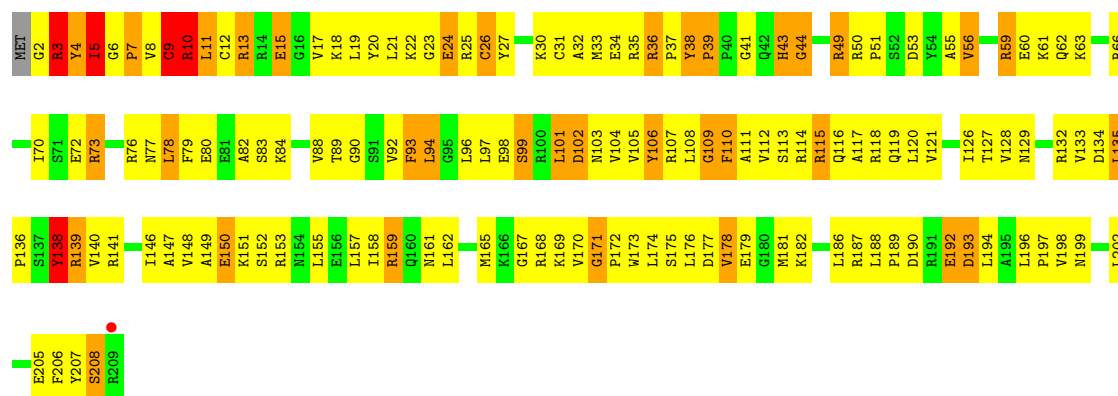






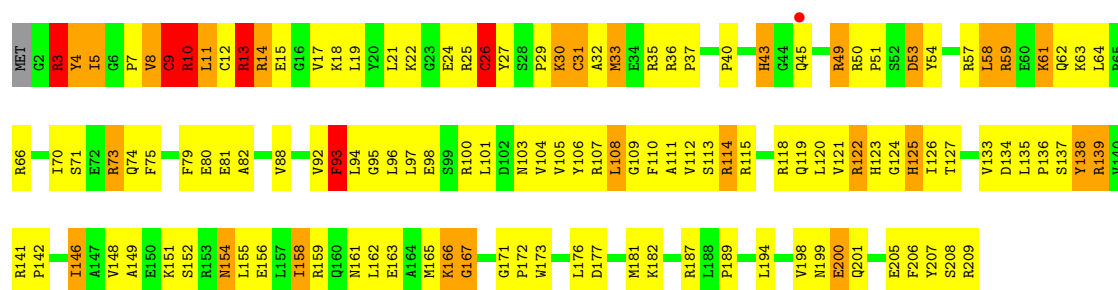
• Molecule 4: 30S ribosomal protein S4

Chain AD:



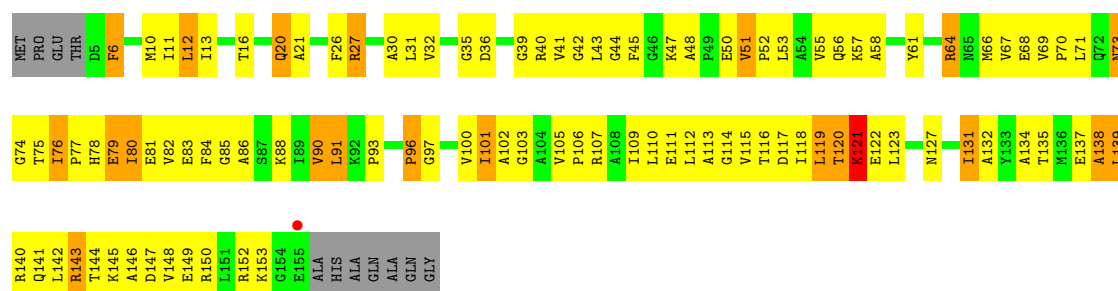
• Molecule 4: 30S ribosomal protein S4

Chain CD:



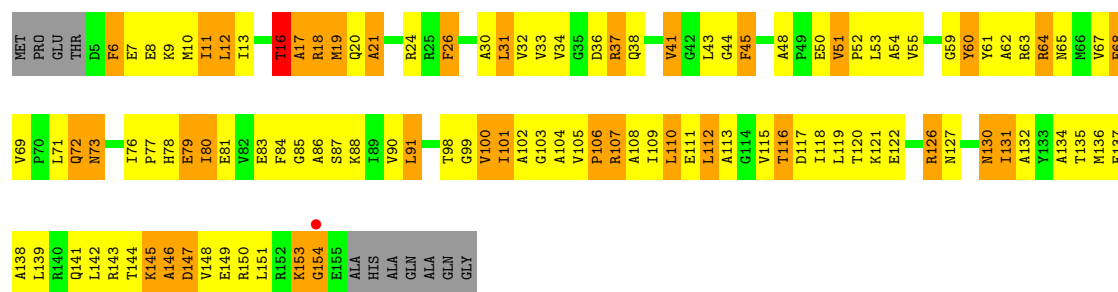
• Molecule 5: 30S ribosomal protein S5

Chain AE:



• Molecule 5: 30S ribosomal protein S5

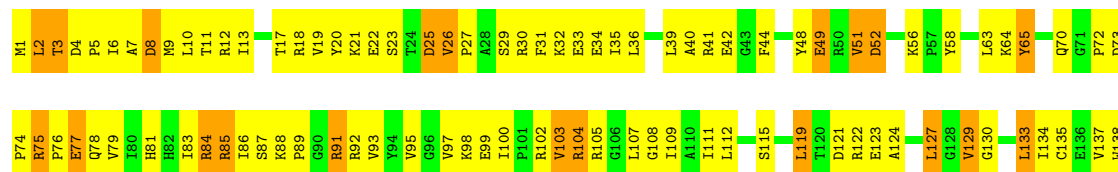
Chain CE:





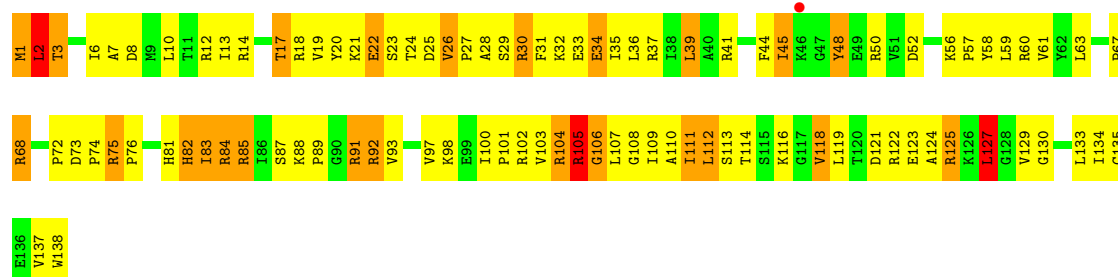
• Molecule 8: 30S ribosomal protein S8

Chain AH:



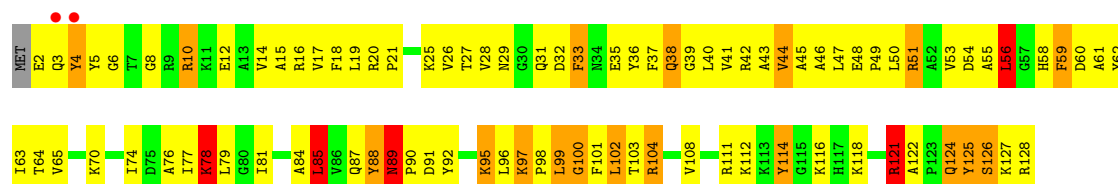
• Molecule 8: 30S ribosomal protein S8

Chain CH:



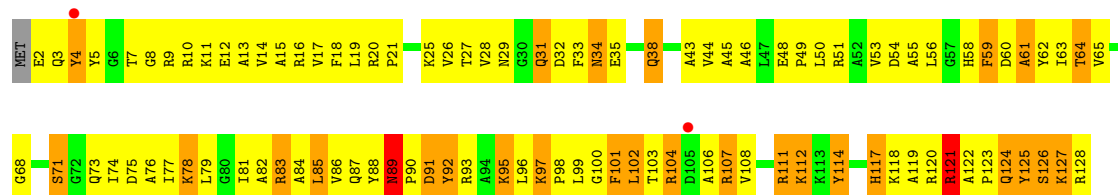
• Molecule 9: 30S ribosomal protein S9

Chain AI:



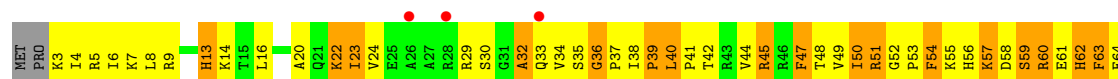
• Molecule 9: 30S ribosomal protein S9

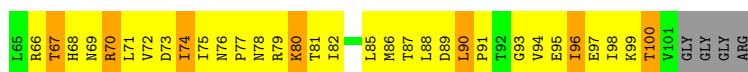
Chain CI:



• Molecule 10: 30S ribosomal protein S10

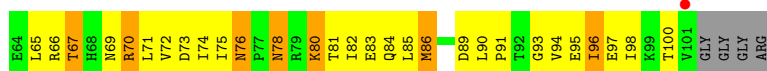
Chain AJ:





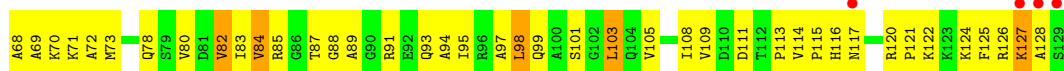
• Molecule 10: 30S ribosomal protein S10

Chain CJ:



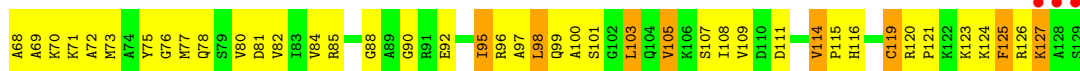
• Molecule 11: 30S ribosomal protein S11

Chain AK:



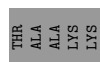
• Molecule 11: 30S ribosomal protein S11

Chain CK:



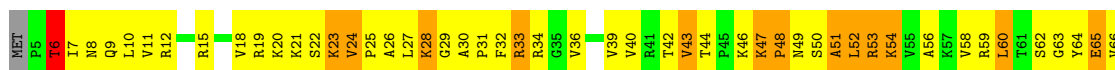
• Molecule 12: 30S ribosomal protein S12

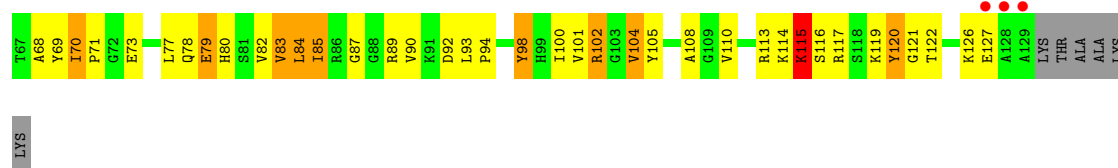
Chain AL:



• Molecule 12: 30S ribosomal protein S12

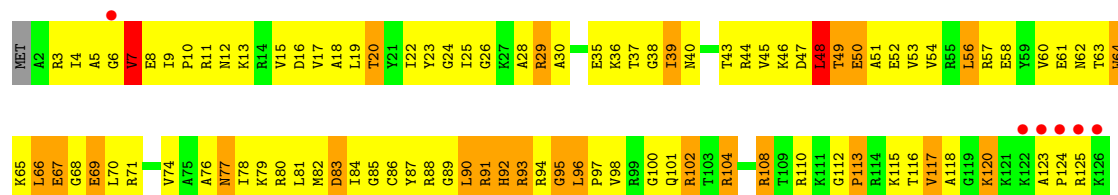
Chain CL:





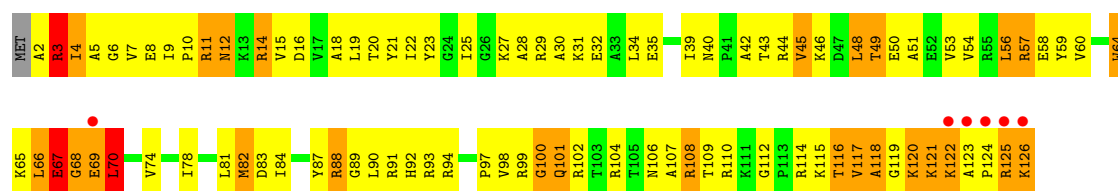
- Molecule 13: 30S ribosomal protein S13

Chain AM:



- Molecule 13: 30S ribosomal protein S13

Chain CM:



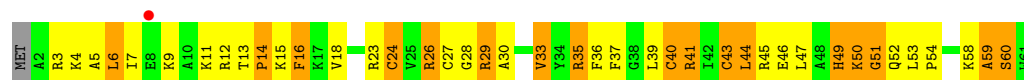
- Molecule 14: 30S ribosomal protein S14 type Z

Chain AN:



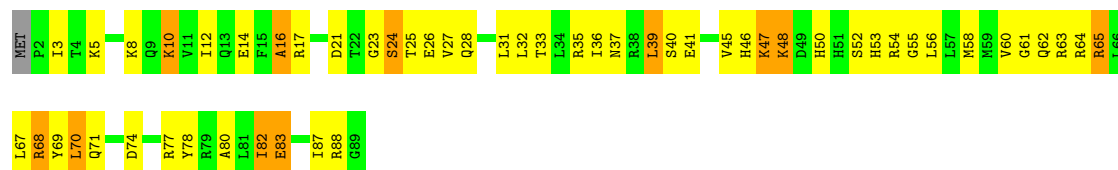
- Molecule 14: 30S ribosomal protein S14 type Z

Chain CN:



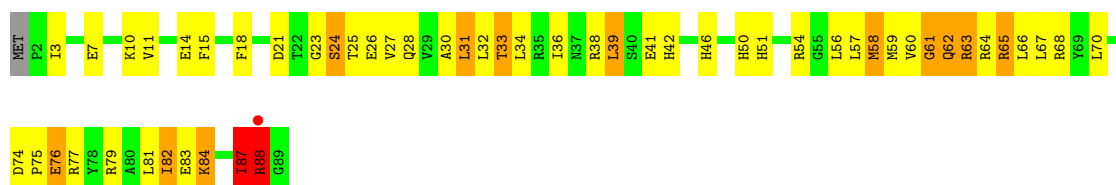
- Molecule 15: 30S ribosomal protein S15

Chain AO:



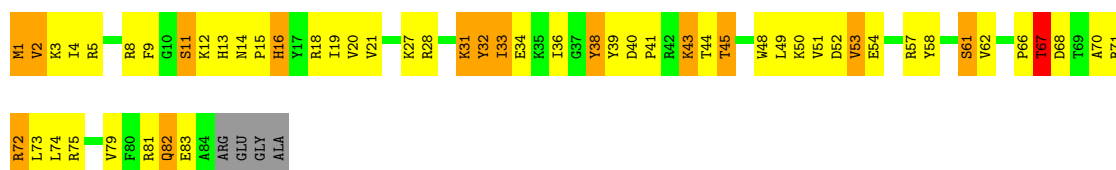
- Molecule 15: 30S ribosomal protein S15

Chain CO:



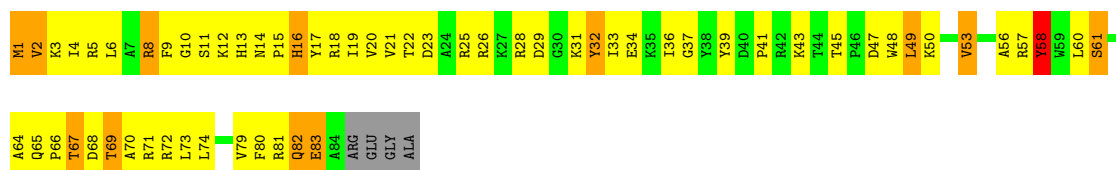
- Molecule 16: 30S ribosomal protein S16

Chain AP:



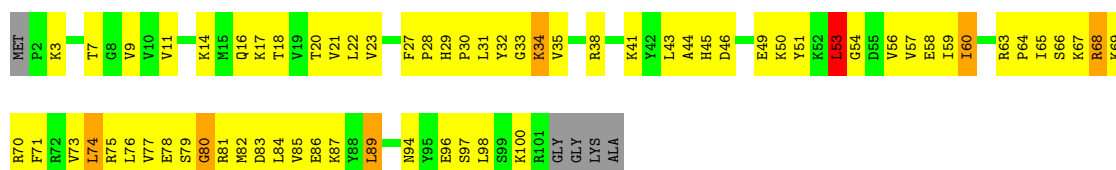
- Molecule 16: 30S ribosomal protein S16

Chain CP:



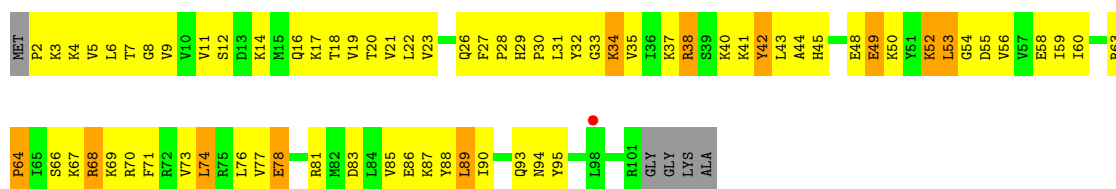
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



- Molecule 17: 30S ribosomal protein S17

Chain CQ:



- Molecule 18: 30S ribosomal protein S18

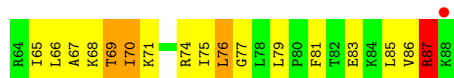
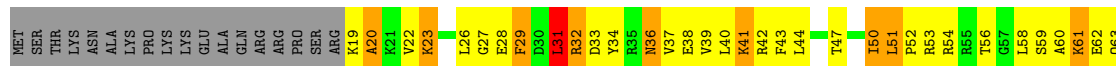
Chain AR:





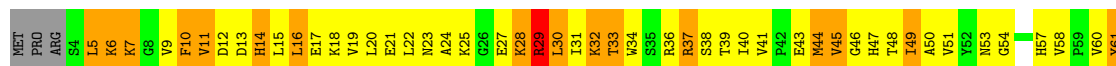
- Molecule 18: 30S ribosomal protein S18

Chain CR:



- Molecule 19: 30S ribosomal protein S19

Chain AS:



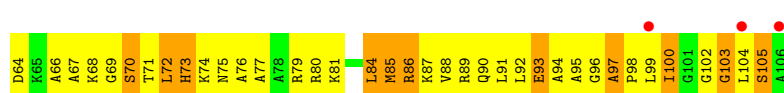
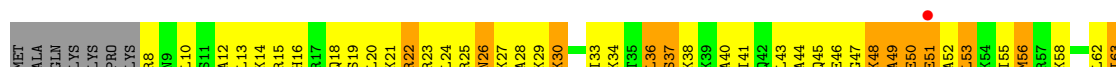
- Molecule 19: 30S ribosomal protein S19

Chain CS:



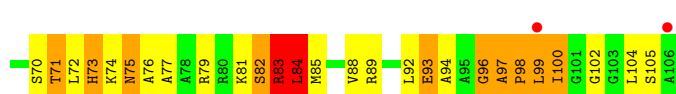
- Molecule 20: 30S ribosomal protein S20

Chain AT:



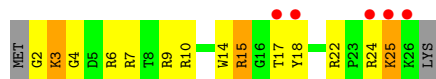
- Molecule 20: 30S ribosomal protein S20

Chain CT:



- Molecule 21: 30S ribosomal protein Thx

Chain AU: 



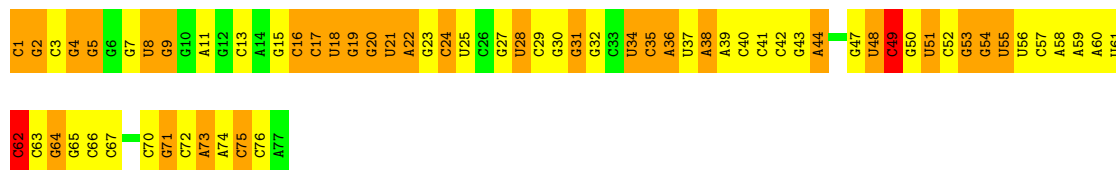
- Molecule 21: 30S ribosomal protein Thx

Chain CU: 



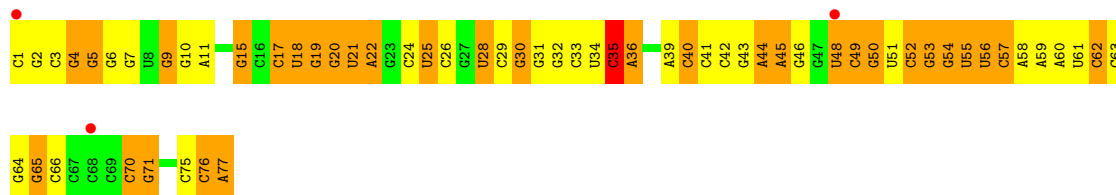
- Molecule 22: P-SITE tRNA fMet

Chain AV: 



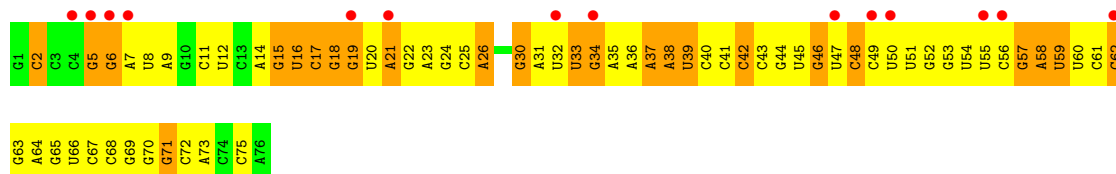
- Molecule 22: P-SITE tRNA fMet

Chain CV: 



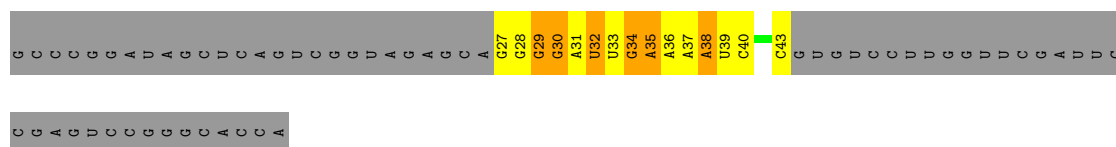
- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe

Chain AW: 



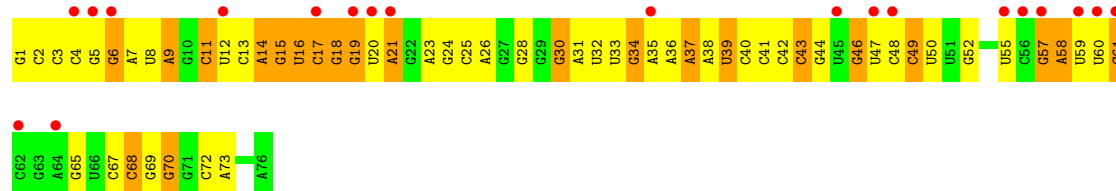
- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe

Chain AY: 



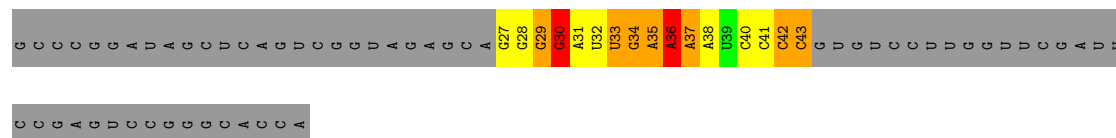
- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe

Chain CW:



- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe

Chain CY:



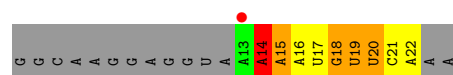
- Molecule 24: mRNA

Chain AX:



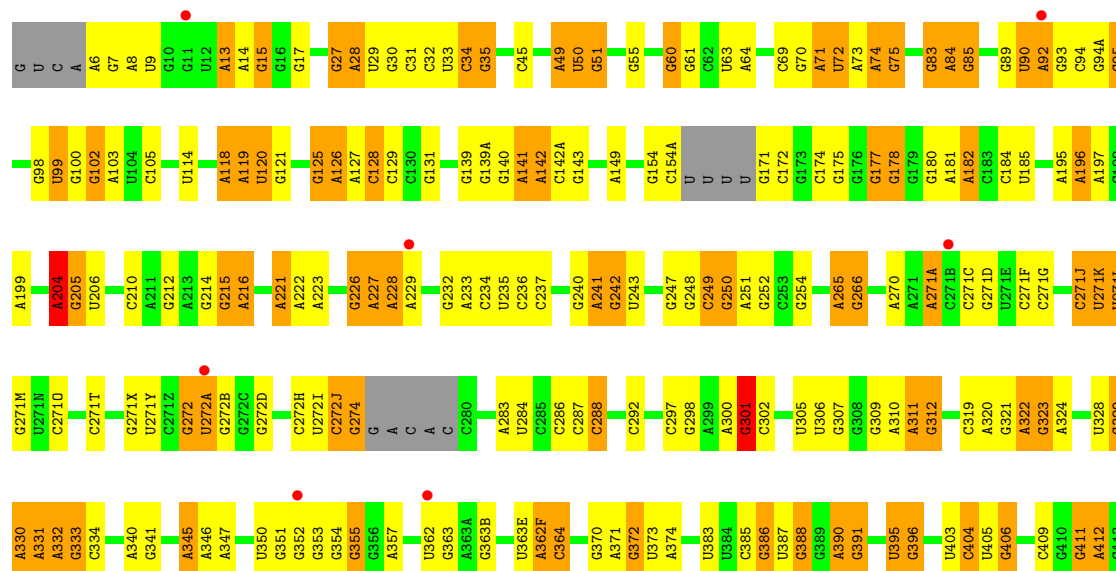
- Molecule 24: mRNA

Chain CX:



- Molecule 25: 23S rRNA

Chain BA:

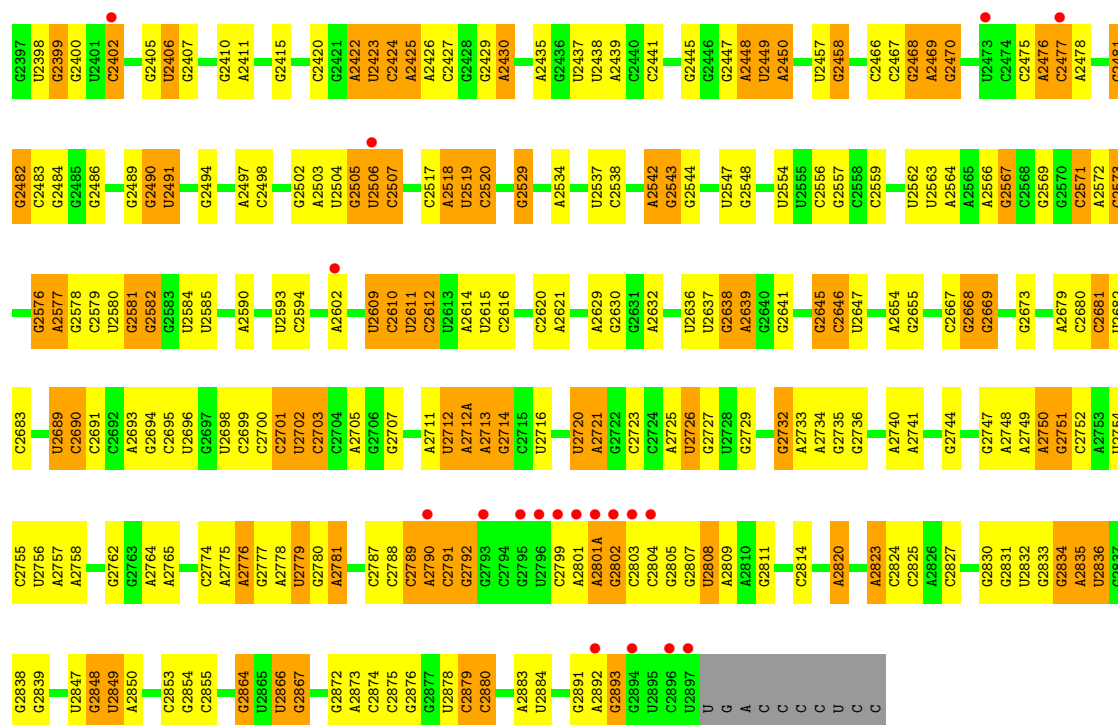


G1524	G1447	G1364	U1288	G1195	A1111	G1051	A980	C893	A800	G711	C589	U504	C414
G1525	G1448	A1365	C1289	G1195	G1112	C1052	A980	A896	G801	G717	A590	A505	A415
G1526	A1449	G1368	C1290	G1203	U1113	C1053	A983	C897	A802	G717	C591	G506	A418
A1528	C1450A	G1368	U1291	G1203	G1114	A	A983	C897	A802	A722	G592	A507	G418
G1532	C1451	A1378	C1297	U1205	G1116	G	G987	A900	A804	A722	G593	C509	A428
G	A1452	A1379	G1298	G1206	G1117	A	G988	A901	G805	U734	G598	G512	A433
U	U1453	G1380	G1299	A1210	C1118	G	G989	C904	C806	G725	C	G	C433
A	G1455	G1384	G1299	U1211	G1122	G	A990	C904	U810	G726	C	U434	U434
C	A1457	U1300	U1300	G1212	U1127	U	C991	U907	U811	A727	G	C517	C435
G1537	C1458	C1386	A1302	A1213	G1126	G	C994	A910	C812	G728	G	G518	C436
G	G1459	C1387	G1303	A1214	A1127	C	A996	A911	U813	G729	C	U519	U519
G1541	A1460	U1390	C1304	A1220	A1128	U	G997	C912	C814	C730	C	G520	G442
A1542	G1461	U1391	C1305	A1220	A1129	U	G997	U913	C817	A734	G	G521	A443
C1543	C1464	A1392	C1306	C1224	U1130	U	A1000	C914	G818	G738	C	G522	A444
A1544	G1465	G1310	G1310	G1224	G1131	A	C1005	A917	A819	G739	G	A526	C445
C1547	C1466	U1311	G1311	G1236	U1132	A	C1006	A918	A820	U740	A	G527	G446
C1548	C1467	U1312	U1312	A1237	U1133	A	C1007	A918	A820	U740	A	A528	U448
C1549	U1396	U1313	G1313	A1237	U1135	G	C1008	A919	U827	A746	A	G529	A449
C1550	A1469	C1314	C1314	A1238	G1136	C	A1009	G921	A829	U747	C	G530	A454
G	G1470	U1397	C1314	A1241	G1139	A	A1010	U922	A830	G749	C	G531	C455
A1554	A1471	C1403	G1319	G1244	U1140	C	G1011	A926	G831	A752	C	G532	C456
G1555	A1472	U1406	C1320	G1244	U1141	C	U1012	A926	G832	A752	C	G533	G457
A1558	G1478	C1407	A1321	G1245	U1142	C	U1013	A926	G833	C753	C	G534	G458
G1560	G1478	U1408	U1322	A1246	A1142	A	U1014	U930	U833	G753	C	A536	U459
G	U1481	G1410	U1324	A1247	A1143	U	G1015	G931	G834	G753	C	C537	A460
A1566	A1482	C1411	G1326	U1249	G1144	C	G1016	G932	G844	U762	C	G546	U464
A1567	G1484	A1412	U1327	G1251	G1149	U	U1017	A933	G845	G763	C	A547	U464
G1568	G1485	G1413	G1328	G1252	C1150	U	U1019	A941	C846	G765	C	A548	G467
A1569	A1486	U1329	A1253	A1252	G1151	A	A1020	G942	U847	G768	C	G549	G468
A1570	G1487	C1330	A1253	A1253	C1153	U	A1021	U943	G848	G769	C	G551	G469
G	G1488	U1331	G1256	G1256	G1154	A	U1022	A944	A849	G769	C	U555	A470
A1572	U1489	G1332	G1264	G1264	U1155	A	G1023	A945	G855	U773	C	G556	G474
G	A1490	C1333	A1265	A1265	A1156	A	G1024	G946	C856	A774	C	A676	U475
U1578	G1491	U1336	U1266	U1266	G1157	U	U1026	G952	C857	G775	C	G559	A478
A1579	C1492	G1337	U1267	U1267	C1161	G	G1027	A953	U858	G776	C	G560	A479
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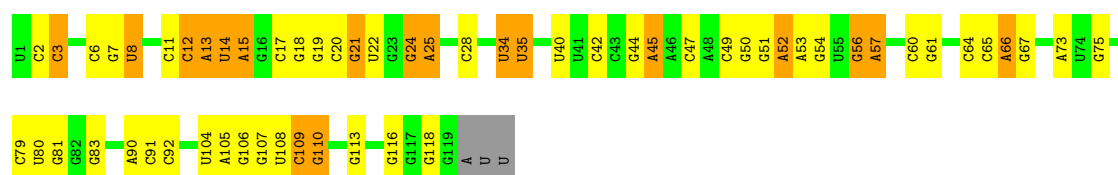


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A2376	G2282	U2098	G2010	A1918	G1817	G1719	G1626	G1537	C1458	G1371	A1286	G1117	
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	G2284	C2103	G2012	G1929	U1819	A1722	G1635	G1541	A1460	G1374	U1288	G1204	
G2382	A2286	G2104	A2013	G1935	A1824	G1744	G1636	A1542	G1465	A1378	C1287	U1206	
G2383	A2287	C2105	A2014	A1936	A1825	G1746	A1637	A1544	C1467	A1379	G1287	G1207	
G2384	A2288	G2106	A2015	A1937	G1826	G1747	A1641	C1547	A1471	U1300	C1208	G1208	
G2385	G2289	C2107	A2016	A1938	G1827	A1747A	G1642	C1548	A1472	A1301	G1209	A1210	
G2386	G2290	C2108	G2018	U1940	A1829	G1748	G1645	C1550	G1473	A1302	G1211	G1212	
U2387	U2291	U2109	A2019	C1941	A1835	A1749	G1646	C1551	G1475	G1303	U1211	G1212	
A2388	G2292	G2110	A2020	A1942	C1836	G1750	C1648	A1554	U1481	G1310	G1218	A1129	
G2389	C2293	G2111	A2021	A1943	C1837	C1751	G1648	A1554	G1482	G1311	G1219		
U2390	U2294	U2112	G2021	U1944	C1838	C1752							
G2391	U2295	U2113	G2022	C1945	C1839	G1753							
A2392	U2296	G2114	A2023	G1946	G1835								
A2393	A2297	C2115	A2024	U1947	C1836								
A2394	G2298	G2116	A2025	U1948	C1837								
G2395	G2299	U2117	A2026	C1949	C1838								
G2396	G2307	A2118	A2027	G1949	G1839								



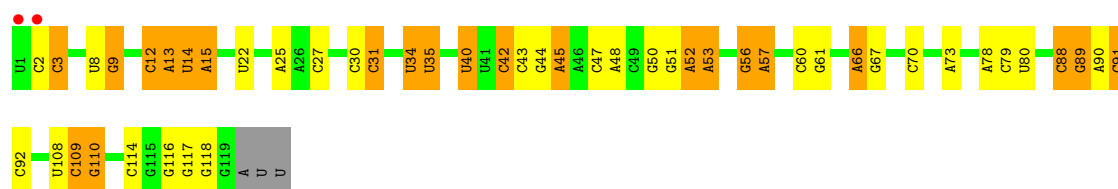
• Molecule 26: 5S rRNA

Chain BB:



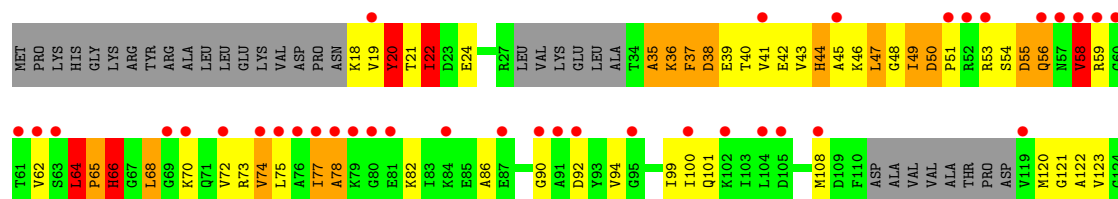
• Molecule 26: 5S rRNA

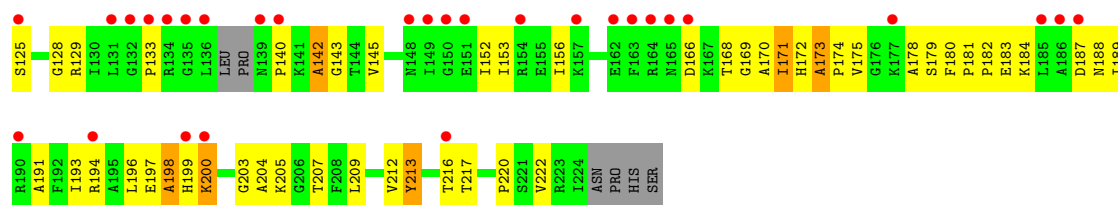
Chain DB:



• Molecule 27: 50S RIBOSOMAL PROTEIN L1

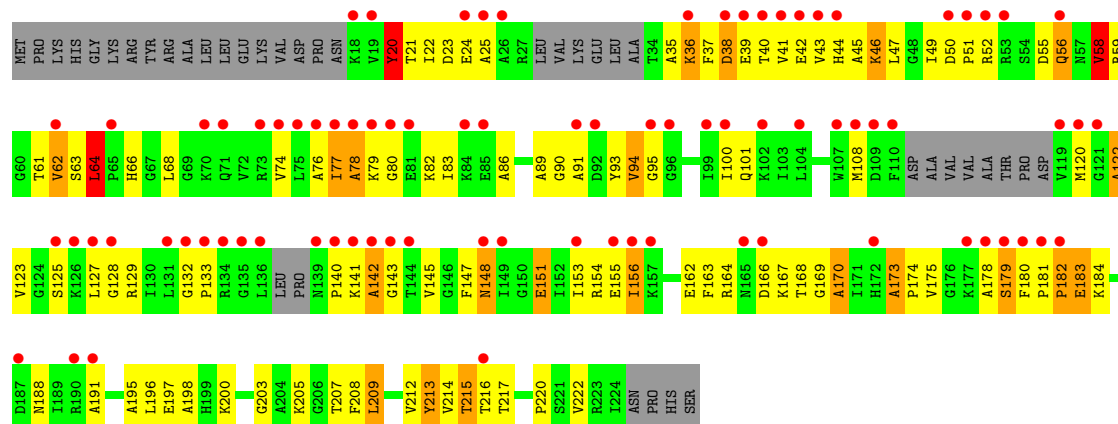
Chain BC:





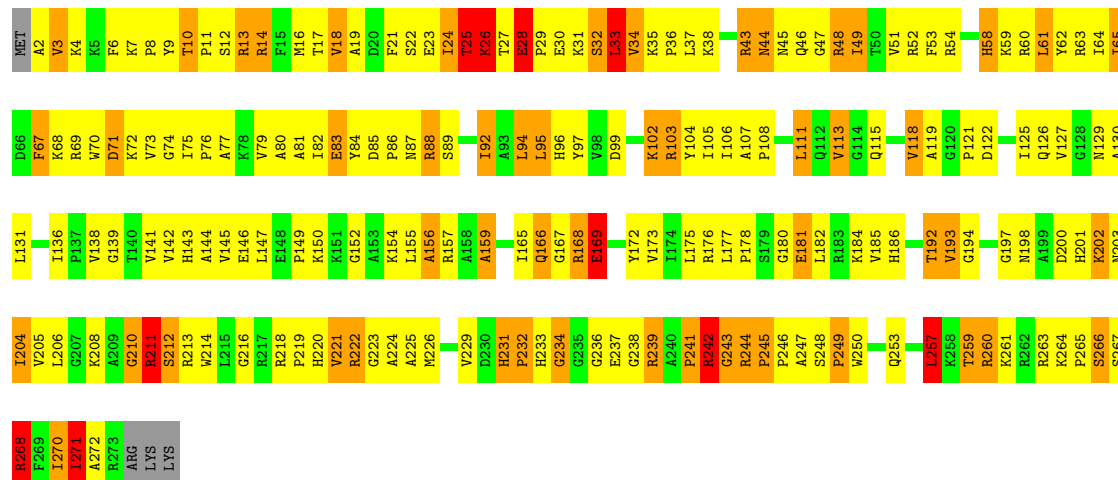
• Molecule 27: 50S RIBOSOMAL PROTEIN L1

Chain DC:



• Molecule 28: 50S RIBOSOMAL PROTEIN L2

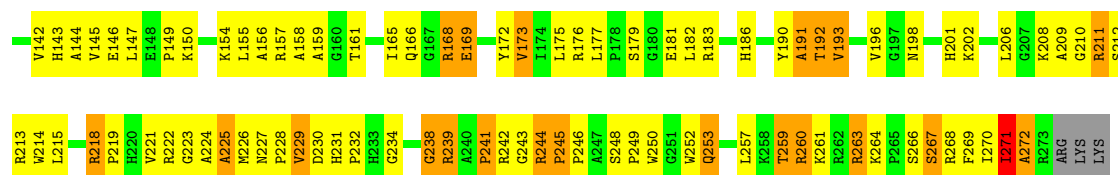
Chain BD:



• Molecule 28: 50S RIBOSOMAL PROTEIN L2

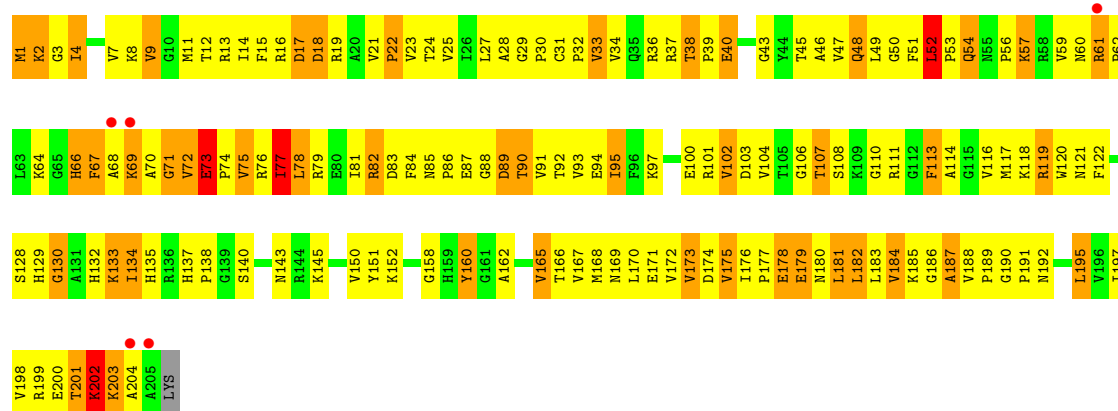
Chain DD:





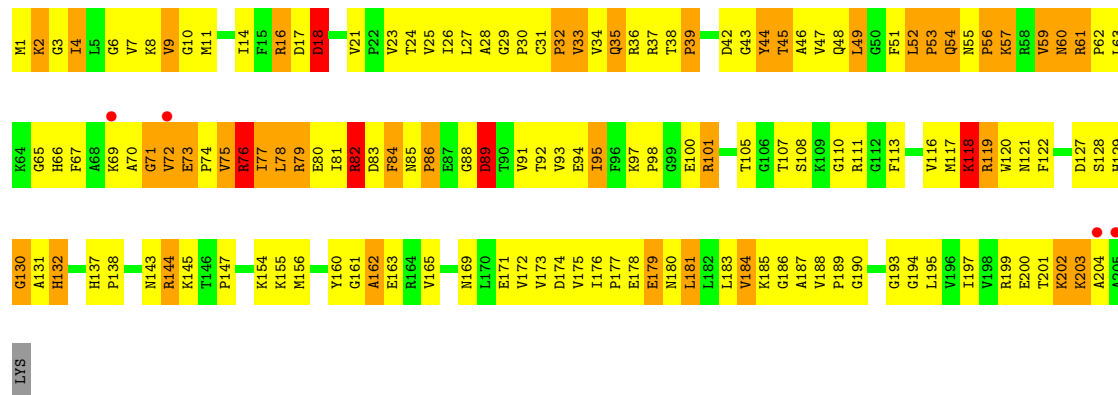
• Molecule 29: 50S RIBOSOMAL PROTEIN L3

Chain BE:



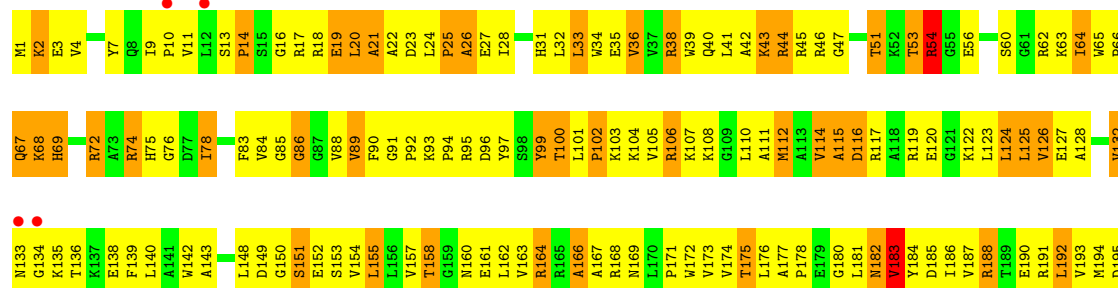
• Molecule 29: 50S RIBOSOMAL PROTEIN L3

Chain DE:



• Molecule 30: 50S RIBOSOMAL PROTEIN L4

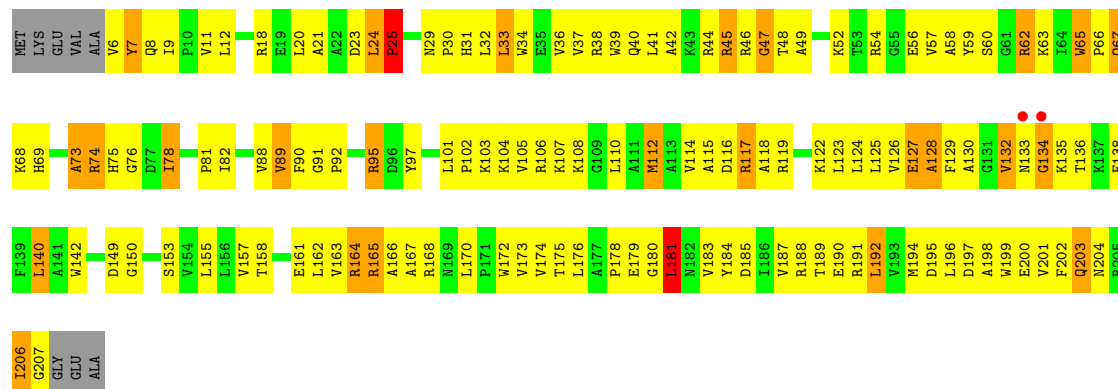
Chain BF:





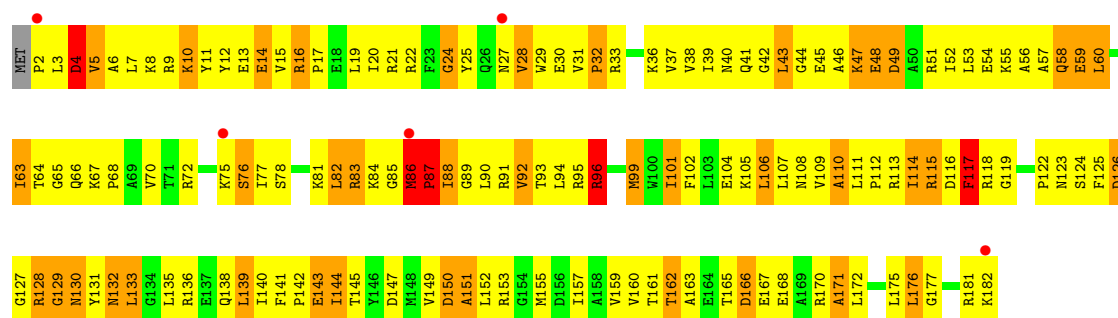
• Molecule 30: 50S RIBOSOMAL PROTEIN L4

Chain DF:



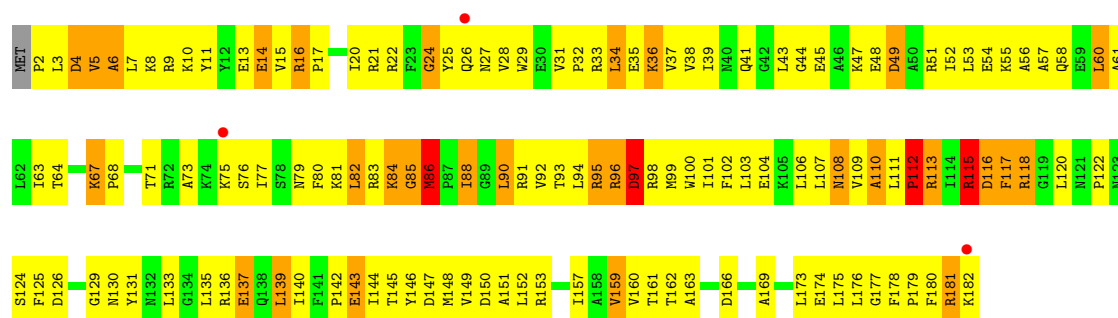
• Molecule 31: 50S RIBOSOMAL PROTEIN L5

Chain BG:



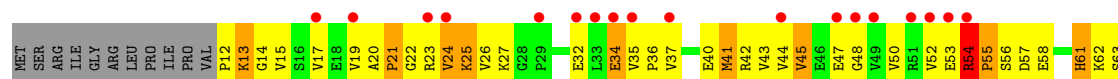
• Molecule 31: 50S RIBOSOMAL PROTEIN L5

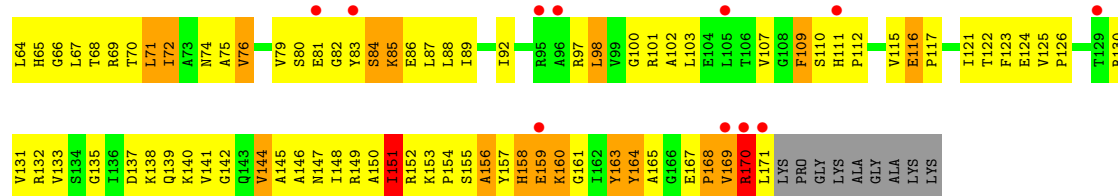
Chain DG:



• Molecule 32: 50S RIBOSOMAL PROTEIN L6

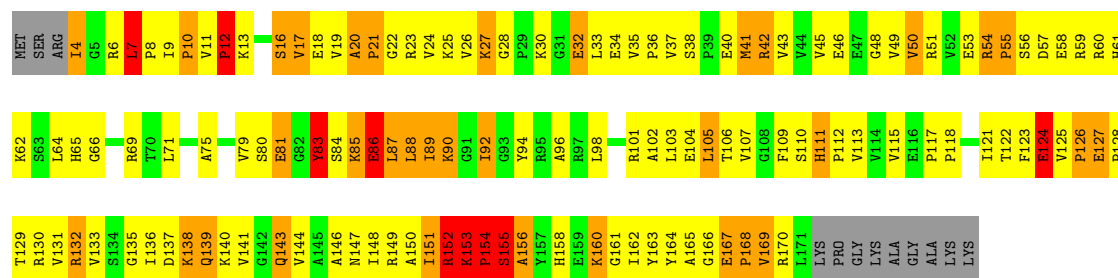
Chain BH:





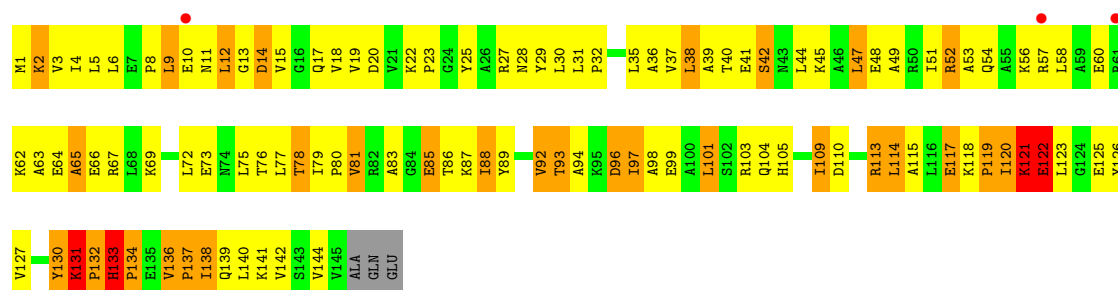
• Molecule 32: 50S RIBOSOMAL PROTEIN L6

Chain DH:



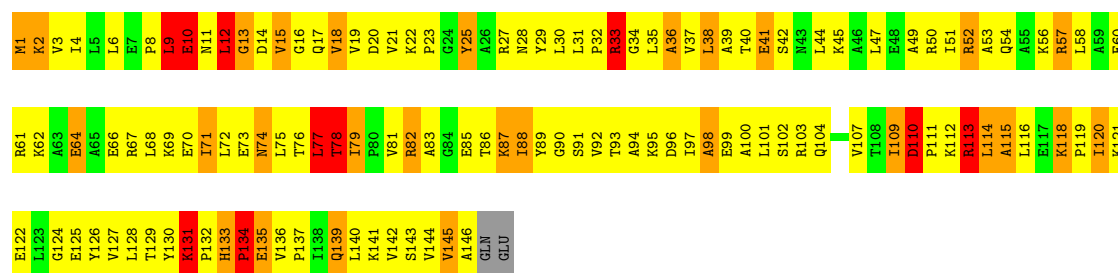
• Molecule 33: 50S RIBOSOMAL PROTEIN L9

Chain BI:



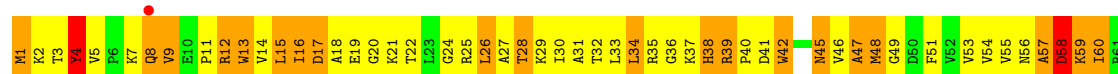
• Molecule 33: 50S RIBOSOMAL PROTEIN L9

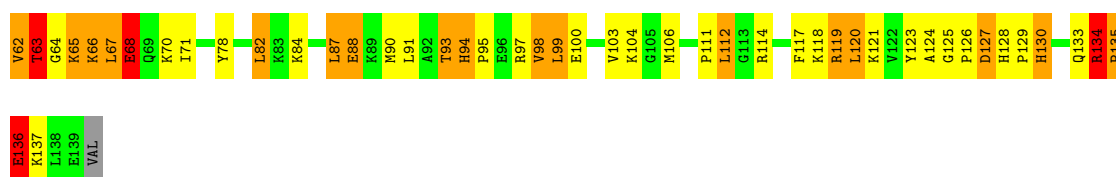
Chain DI:



• Molecule 34: 50S RIBOSOMAL PROTEIN L13

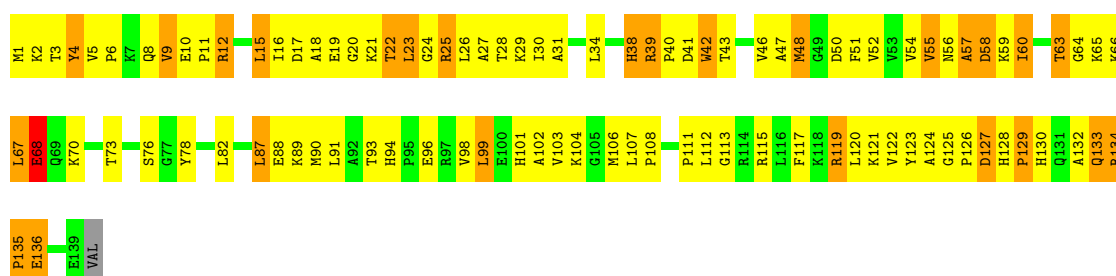
Chain BN:





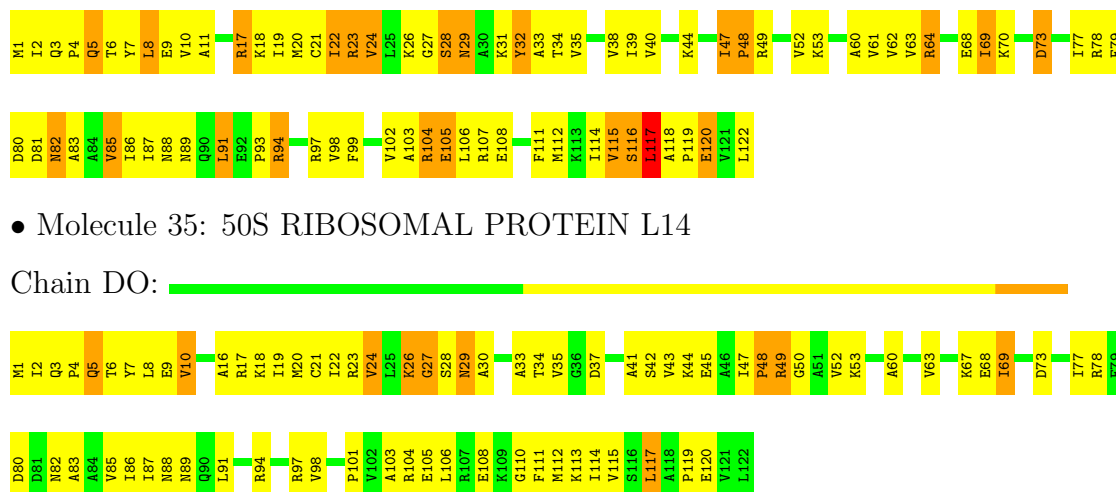
• Molecule 34: 50S RIBOSOMAL PROTEIN L13

Chain DN:



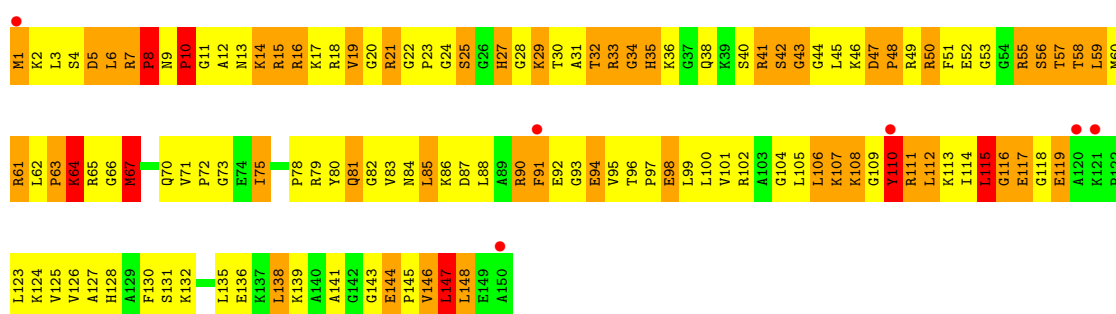
• Molecule 35: 50S RIBOSOMAL PROTEIN L14

Chain BO:



• Molecule 35: 50S RIBOSOMAL PROTEIN L14

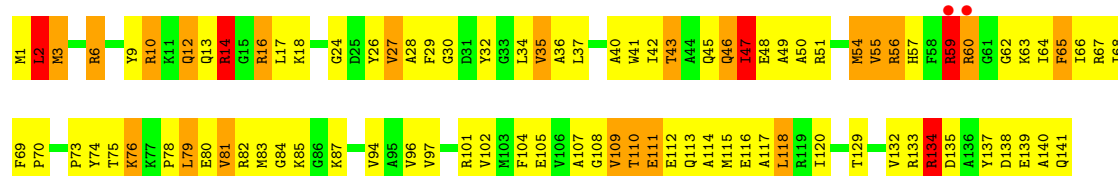
Chain DO:



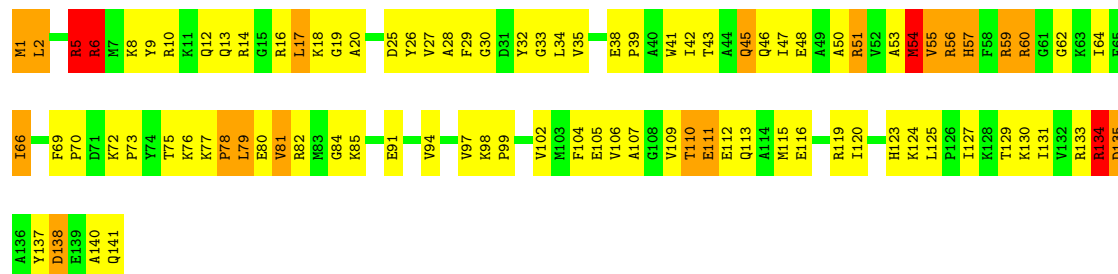
• Molecule 36: 50S RIBOSOMAL PROTEIN L15

V125	P63	H1
V126	P64	K2
A127	R65	L3
H128	G66	S4
A129	P67	D5
F130	Q70	L6
S131	V71	R7
K132	P72	P8
L135	G73	N9
E136	F74	P10
K137	I75	G11
L138	P78	A12
K139	R79	M13
A140	Y80	K14
A141	O81	R16
G142	G82	K17
G143	H83	R18
E144	N84	V19
P145	L85	G20
V146	K86	R21
L147	D87	G22
L148	L88	P23
E149	A89	G24
A150	R90	H27
	F91	G28
	E92	K29
	G93	T30
	E94	A31
	V95	T32
	T96	R33
	P97	G34
	E98	H35
	L99	K36
	L100	G37
	V101	Q38
	R102	L
	A103	R41
	G104	S42
	L105	G43
	L106	G44
	K107	L45
	K108	K46
	G109	D47
	V110	P48
	R111	R49
	L112	R50
	K113	F51
	L114	E52
	L115	G53
	G116	G54
	E117	R55
	G118	S56
	E119	T57
	A120	T58
	K121	L59
	P122	M60
	L123	R61
	V124	L62

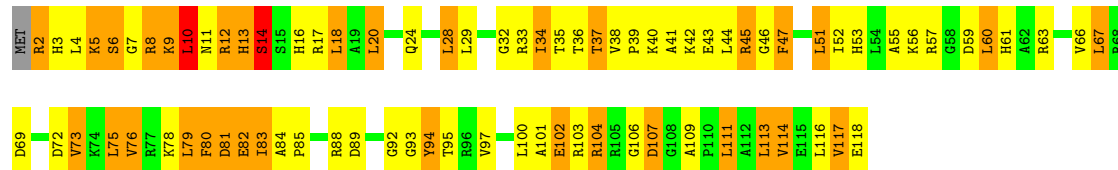
Chain BQ:



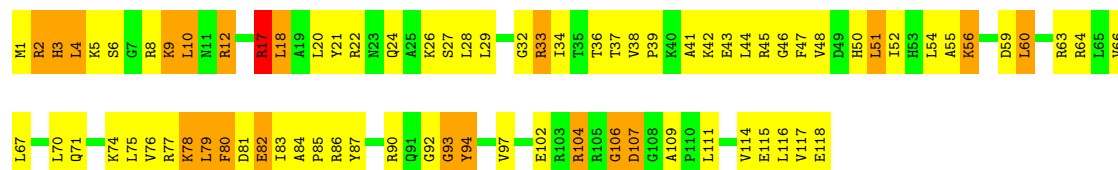
Chain DQ:



Chain BR:

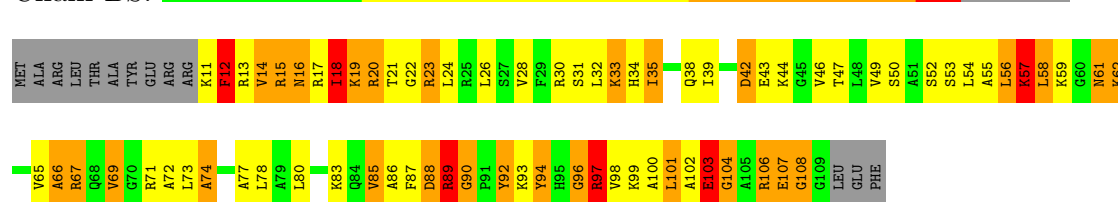


Chain DR:



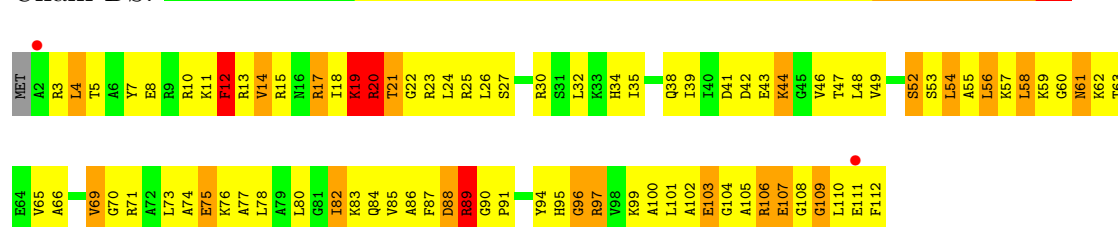
- Molecule 39: 50S RIBOSOMAL PROTEIN L18

Chain BS:



- Molecule 39: 50S RIBOSOMAL PROTEIN L18

Chain DS:



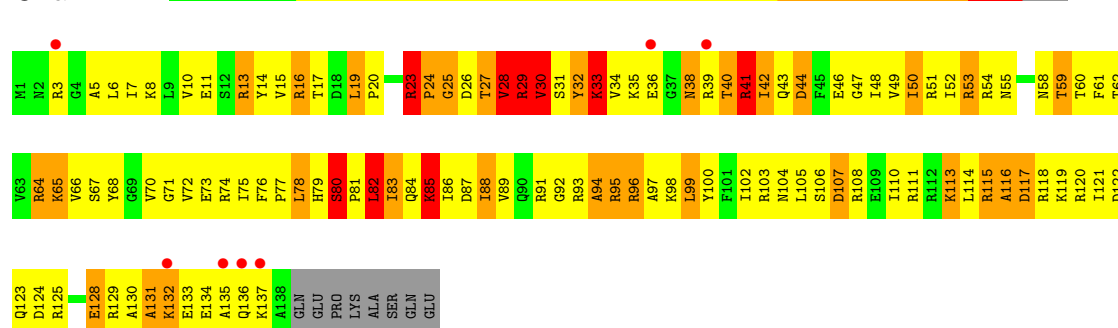
- Molecule 40: 50S RIBOSOMAL PROTEIN L19

Chain BT:



- Molecule 40: 50S RIBOSOMAL PROTEIN L19

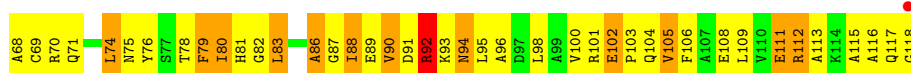
Chain DT:



- Molecule 41: 50S RIBOSOMAL PROTEIN L20

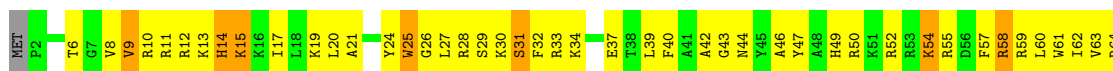
Chain BU:





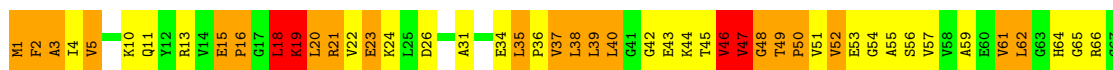
• Molecule 41: 50S RIBOSOMAL PROTEIN L20

Chain DU:



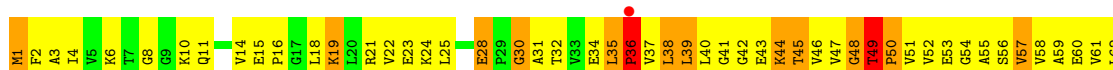
• Molecule 42: 50S RIBOSOMAL PROTEIN L21

Chain BV:



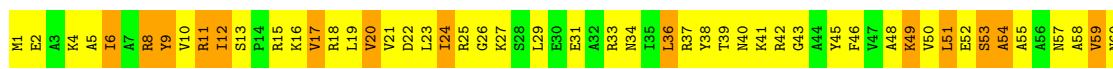
• Molecule 42: 50S RIBOSOMAL PROTEIN L21

Chain DV:



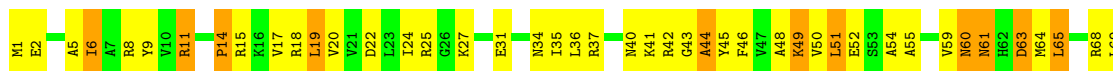
• Molecule 43: 50S RIBOSOMAL PROTEIN L22

Chain BW:



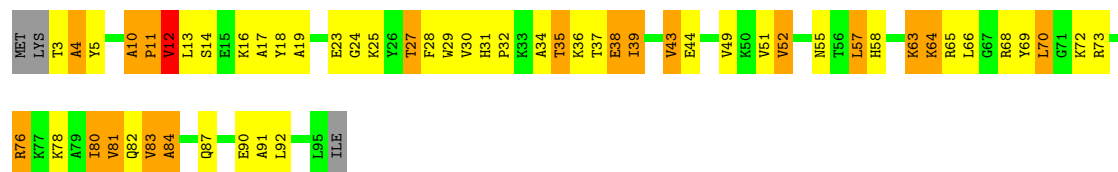
• Molecule 43: 50S RIBOSOMAL PROTEIN L22

Chain DW:



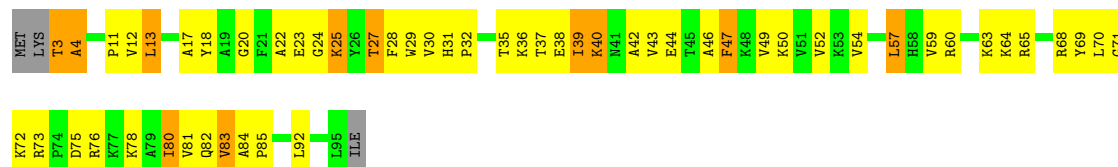
• Molecule 44: 50S RIBOSOMAL PROTEIN L23

Chain BX:



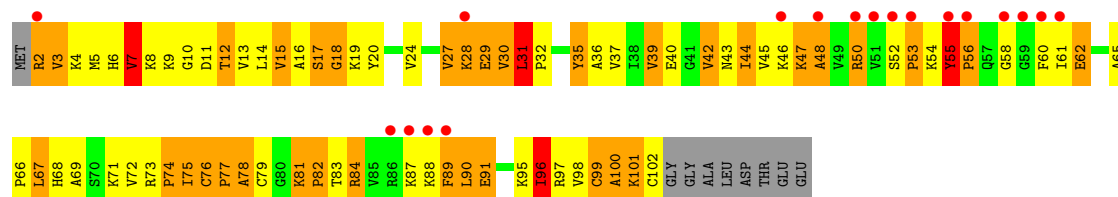
- Molecule 44: 50S RIBOSOMAL PROTEIN L23

Chain DX:



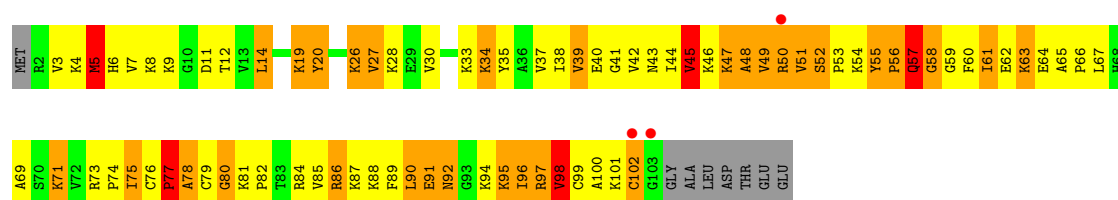
- Molecule 45: 50S RIBOSOMAL PROTEIN L24

Chain BY:



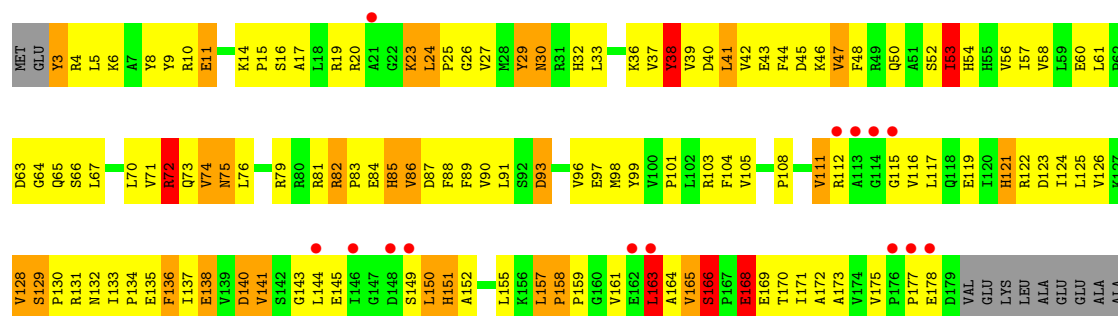
- Molecule 45: 50S RIBOSOMAL PROTEIN L24

Chain DY:



- Molecule 46: 50S RIBOSOMAL PROTEIN L25

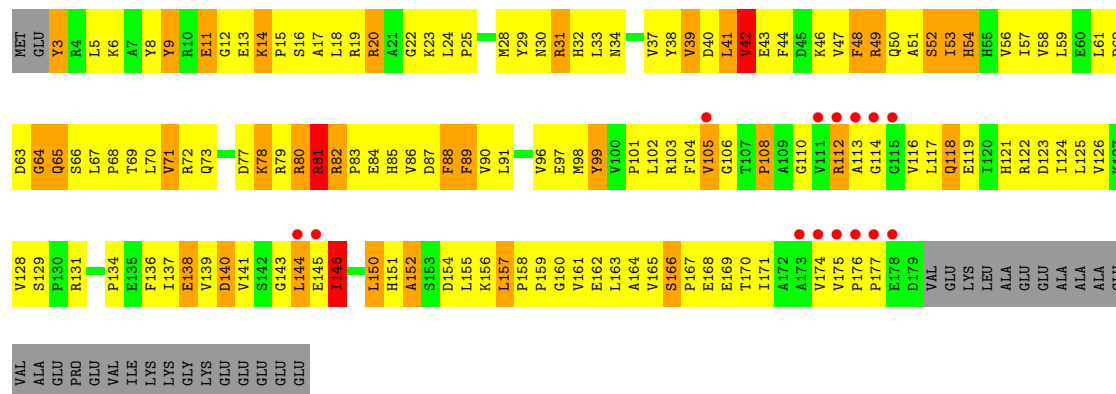
Chain BZ:



ALA
GLU
VAL
ALA
GLU
PRO
GLU
VAL
ILE
LYS
LYS
GLY
LYS
GLU
GLU
GLU
GLU

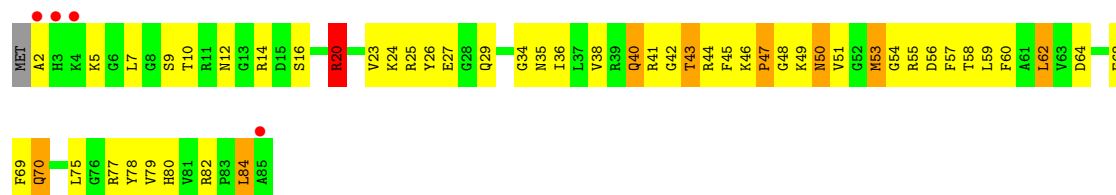
• Molecule 46: 50S RIBOSOMAL PROTEIN L25

Chain DZ:



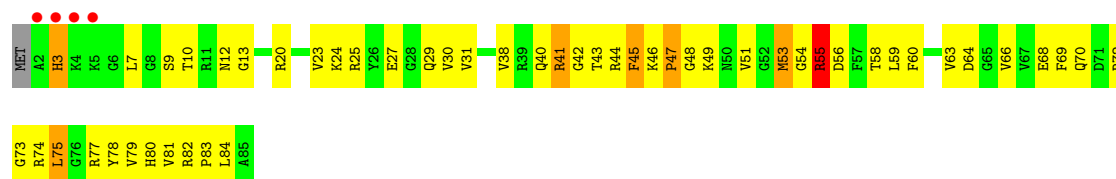
• Molecule 47: 50S RIBOSOMAL PROTEIN L27

Chain B0:



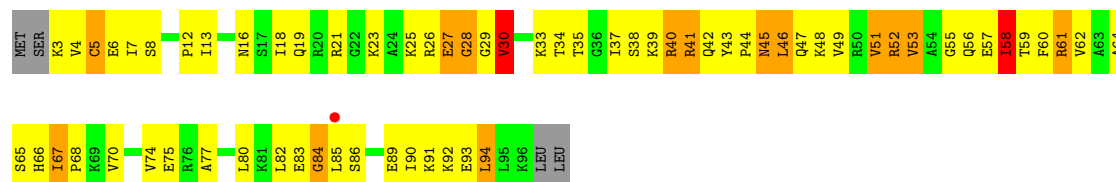
• Molecule 47: 50S RIBOSOMAL PROTEIN L27

Chain D0:



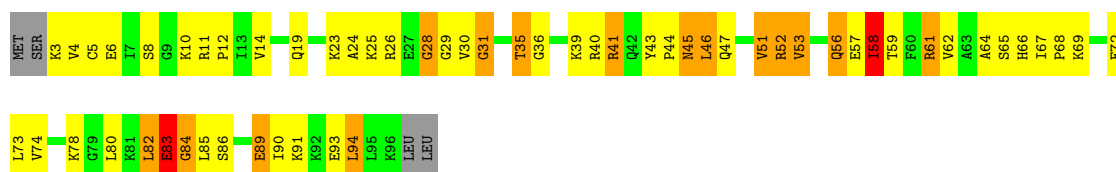
• Molecule 48: 50S RIBOSOMAL PROTEIN L28

Chain B1:



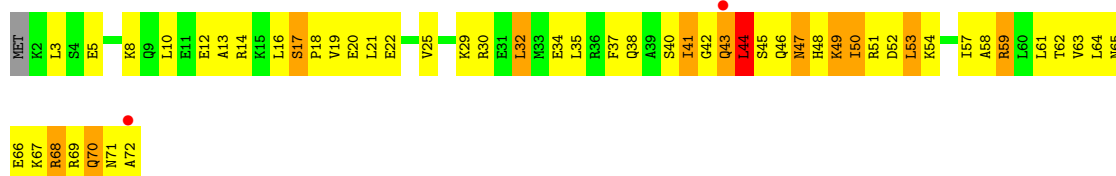
• Molecule 48: 50S RIBOSOMAL PROTEIN L28

Chain D1:



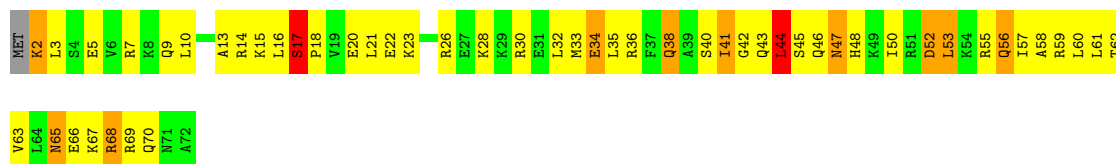
• Molecule 49: 50S RIBOSOMAL PROTEIN L29

Chain B2:



• Molecule 49: 50S RIBOSOMAL PROTEIN L29

Chain D2:



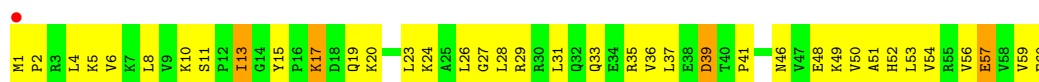
• Molecule 50: 50S RIBOSOMAL PROTEIN L30

Chain B3:



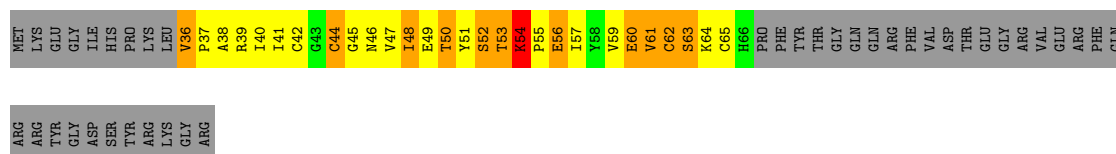
• Molecule 50: 50S RIBOSOMAL PROTEIN L30

Chain D3:



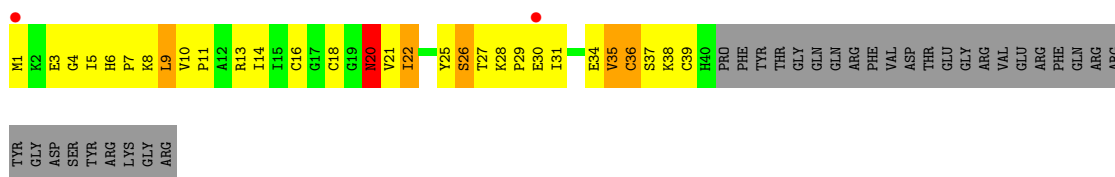
• Molecule 51: 50S RIBOSOMAL PROTEIN L31

Chain B4:



• Molecule 51: 50S RIBOSOMAL PROTEIN L31

Chain D4:



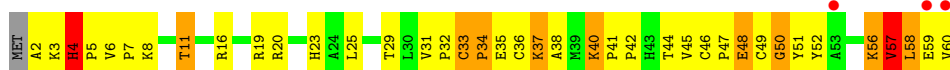
• Molecule 52: 50S RIBOSOMAL PROTEIN L32

Chain B5:



• Molecule 52: 50S RIBOSOMAL PROTEIN L32

Chain D5:



• Molecule 53: 50S RIBOSOMAL PROTEIN L33

Chain B6:



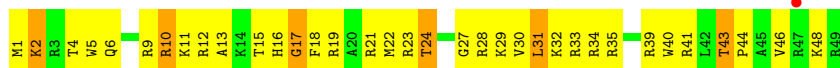
• Molecule 53: 50S RIBOSOMAL PROTEIN L33

Chain D6:



• Molecule 54: 50S RIBOSOMAL PROTEIN L34

Chain B7:



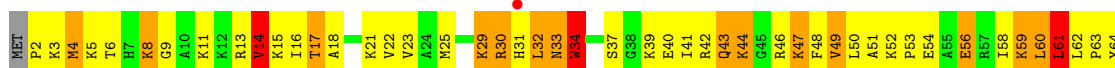
• Molecule 54: 50S RIBOSOMAL PROTEIN L34

Chain D7:



• Molecule 55: 50S RIBOSOMAL PROTEIN L35

Chain B8:



B65

• Molecule 55: 50S RIBOSOMAL PROTEIN L35

Chain D8:



B65

• Molecule 56: 50S RIBOSOMAL PROTEIN L36

Chain B9:



• Molecule 56: 50S RIBOSOMAL PROTEIN L36

Chain D9:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.46Å 447.34Å 622.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.07 – 3.52 35.07 – 3.52	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.07-3.52) 99.9 (35.07-3.52)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	0.46	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.47Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1069)	Depositor
R, R_{free}	0.210 , 0.249 0.216 , 0.255	Depositor DCC
R_{free} test set	32826 reflections (4.78%)	DCC
Wilson B-factor (Å ²)	91.1	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 36.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 720017 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	293977	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, PAR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.28	0/36189	0.82	11/56484 (0.0%)
1	CA	0.29	0/36189	0.82	14/56484 (0.0%)
2	AB	0.59	0/1936	0.68	0/2611
2	CB	0.67	0/1936	0.77	0/2611
3	AC	0.70	0/1637	0.76	0/2207
3	CC	0.73	0/1637	0.82	0/2207
4	AD	0.69	0/1733	0.80	0/2318
4	CD	0.77	1/1733 (0.1%)	0.85	0/2318
5	AE	0.71	0/1163	0.88	0/1566
5	CE	0.74	0/1163	0.84	0/1566
6	AF	0.73	0/856	0.89	0/1154
6	CF	0.79	0/856	0.82	0/1154
7	AG	0.72	0/1276	0.79	0/1709
7	CG	0.71	0/1276	0.77	0/1709
8	AH	0.69	1/1136 (0.1%)	0.78	0/1527
8	CH	0.73	0/1136	0.80	1/1527 (0.1%)
9	AI	0.71	0/1029	0.80	0/1379
9	CI	0.70	0/1029	0.81	1/1379 (0.1%)
10	AJ	0.70	0/808	0.79	0/1087
10	CJ	0.65	0/808	0.77	0/1087
11	AK	0.67	0/900	0.81	0/1213
11	CK	0.70	0/900	0.82	0/1213
12	AL	0.86	0/987	0.95	0/1322
12	CL	0.92	1/987 (0.1%)	1.01	0/1322
13	AM	0.67	0/999	0.82	0/1338
13	CM	0.48	1/1008 (0.1%)	0.75	1/1347 (0.1%)
14	AN	0.73	0/501	0.83	1/664 (0.2%)
14	CN	0.77	0/501	0.95	0/664
15	AO	0.72	0/745	0.79	0/992
15	CO	0.71	0/745	0.81	0/992
16	AP	0.72	0/717	0.86	0/965
16	CP	0.79	0/717	0.84	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.69	0/837	0.79	0/1119
17	CQ	0.73	0/837	0.81	0/1119
18	AR	0.69	0/579	0.83	0/768
18	CR	0.76	0/579	0.98	0/768
19	AS	0.66	0/643	0.76	0/867
19	CS	0.80	1/643 (0.2%)	0.86	0/867
20	AT	0.73	0/765	0.77	0/1007
20	CT	0.61	0/765	0.63	0/1007
21	AU	0.73	0/213	0.83	0/279
21	CU	0.75	0/213	0.78	0/279
22	AV	1.13	5/1836 (0.3%)	1.33	13/2859 (0.5%)
22	CV	1.02	0/1835	1.20	13/2859 (0.5%)
23	AW	0.93	3/1809 (0.2%)	1.07	4/2819 (0.1%)
23	AY	1.07	1/408 (0.2%)	1.39	4/634 (0.6%)
23	CW	0.90	0/1809	1.01	0/2819
23	CY	1.15	0/408	1.42	4/634 (0.6%)
24	AX	1.10	1/285 (0.4%)	0.91	2/441 (0.5%)
24	CX	0.96	0/235	1.27	3/364 (0.8%)
25	BA	0.34	1/67788 (0.0%)	0.87	42/105819 (0.0%)
25	DA	0.35	0/68124	0.88	36/106343 (0.0%)
26	BB	0.26	0/2853	0.78	0/4451
26	DB	0.28	0/2853	0.80	0/4451
27	BC	0.65	1/1145 (0.1%)	0.67	0/1556
27	DC	0.24	0/1145	0.46	0/1556
28	BD	0.85	0/2155	0.95	1/2907 (0.0%)
28	DD	0.54	0/2155	0.74	0/2907
29	BE	0.75	0/1597	0.89	0/2155
29	DE	0.49	1/1597 (0.1%)	0.72	0/2155
30	BF	0.80	0/1659	0.87	1/2246 (0.0%)
30	DF	0.49	0/1620	0.76	1/2194 (0.0%)
31	BG	0.70	0/1499	0.78	1/2016 (0.0%)
31	DG	0.42	1/1499 (0.1%)	0.68	1/2016 (0.0%)
32	BH	0.63	0/1246	0.69	0/1684
32	DH	0.40	0/1315	0.79	1/1780 (0.1%)
33	BI	0.67	0/1146	0.81	0/1551
33	DI	0.36	0/1151	0.74	1/1558 (0.1%)
34	BN	0.76	0/1132	0.83	0/1527
34	DN	0.43	0/1132	0.69	0/1527
35	BO	0.76	0/943	0.87	0/1269
35	DO	0.46	0/943	0.68	0/1269
36	BP	0.40	1/1162 (0.1%)	0.78	2/1544 (0.1%)
36	DP	0.39	0/1162	0.76	1/1544 (0.1%)
37	BQ	0.75	0/1143	0.87	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DQ	0.48	0/1143	0.65	0/1527
38	BR	0.80	0/974	0.90	1/1302 (0.1%)
38	DR	0.57	1/982 (0.1%)	0.79	2/1312 (0.2%)
39	BS	0.77	0/779	0.90	0/1038
39	DS	0.40	0/892	0.81	1/1187 (0.1%)
40	BT	0.71	0/1156	0.90	1/1544 (0.1%)
40	DT	0.56	1/1156 (0.1%)	0.84	6/1544 (0.4%)
41	BU	0.81	0/982	0.91	1/1306 (0.1%)
41	DU	0.51	0/975	0.75	0/1297
42	BV	0.72	0/790	0.90	1/1057 (0.1%)
42	DV	0.53	1/790 (0.1%)	0.82	0/1057
43	BW	0.81	0/907	0.89	1/1216 (0.1%)
43	DW	0.48	0/907	0.69	1/1216 (0.1%)
44	BX	0.75	0/740	0.89	1/995 (0.1%)
44	DX	0.52	0/740	0.68	0/995
45	BY	0.74	0/789	0.95	2/1053 (0.2%)
45	DY	0.55	2/798 (0.3%)	0.78	0/1064
46	BZ	0.72	0/1436	0.74	1/1951 (0.1%)
46	DZ	0.35	0/1436	0.57	0/1951
47	B0	0.79	1/671 (0.1%)	0.84	0/892
47	D0	0.44	0/671	0.64	0/892
48	B1	0.87	0/739	0.94	0/983
48	D1	0.48	0/739	0.73	0/983
49	B2	0.72	0/600	0.83	0/793
49	D2	0.54	0/600	0.71	0/793
50	B3	0.73	0/473	0.83	0/636
50	D3	0.43	0/473	0.71	0/636
51	B4	0.72	0/229	0.76	0/311
51	D4	0.40	0/303	0.70	0/409
52	B5	0.82	1/473 (0.2%)	0.83	0/639
52	D5	0.44	0/473	0.65	0/639
53	B6	0.67	0/388	0.92	0/520
53	D6	0.30	0/388	0.58	0/520
54	B7	0.88	0/427	0.99	0/563
54	D7	0.54	0/427	0.75	1/563 (0.2%)
55	B8	0.76	0/516	0.91	0/681
55	D8	0.51	0/516	0.82	0/681
56	B9	0.64	0/302	0.59	0/397
56	D9	0.26	0/302	0.46	0/397
All	All	0.48	27/318178 (0.0%)	0.85	180/475682 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
28	BD	0	1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1453	U	O3'-P	29.98	1.97	1.61
24	AX	14	A	O3'-P	-13.06	1.45	1.61
38	DR	12	ARG	C-N	11.33	1.60	1.34
40	DT	28	VAL	C-N	10.90	1.59	1.34
22	AV	1	C	OP3-P	-9.31	1.50	1.61

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	1453	U	P-O3'-C3'	-10.66	106.91	119.70
38	DR	12	ARG	O-C-N	9.52	137.93	122.70
36	BP	1	MET	CG-SD-CE	9.44	115.30	100.20
40	DT	28	VAL	O-C-N	8.73	136.67	122.70
40	DT	28	VAL	CA-C-N	-7.49	100.72	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	BD	222	ARG	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32328	0	16317	795	0
1	CA	32328	0	16317	871	1
2	AB	1901	0	1951	245	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CB	1901	0	1951	232	0
3	AC	1613	0	1677	197	0
3	CC	1613	0	1677	148	0
4	AD	1703	0	1765	191	0
4	CD	1703	0	1764	174	0
5	AE	1147	0	1207	148	0
5	CE	1147	0	1207	159	0
6	AF	843	0	857	87	0
6	CF	843	0	857	63	0
7	AG	1257	0	1296	123	0
7	CG	1257	0	1296	102	0
8	AH	1116	0	1177	111	0
8	CH	1116	0	1177	111	0
9	AI	1010	0	1037	133	0
9	CI	1010	0	1037	144	0
10	AJ	795	0	840	127	0
10	CJ	795	0	840	135	0
11	AK	885	0	904	97	0
11	CK	885	0	904	109	0
12	AL	971	0	1057	126	0
12	CL	971	0	1057	123	0
13	AM	988	0	1059	151	0
13	CM	997	0	1072	164	0
14	AN	492	0	529	87	0
14	CN	492	0	531	69	0
15	AO	734	0	771	61	0
15	CO	734	0	771	51	0
16	AP	701	0	720	62	0
16	CP	701	0	720	101	0
17	AQ	824	0	891	68	0
17	CQ	824	0	891	85	0
18	AR	574	0	644	62	0
18	CR	574	0	644	68	0
19	AS	630	0	652	117	0
19	CS	630	0	652	106	0
20	AT	763	0	861	132	0
20	CT	763	0	861	166	0
21	AU	209	0	221	12	0
21	CU	209	0	221	22	0
22	AV	1644	0	836	110	0
22	CV	1643	0	836	143	0
23	AW	1619	0	822	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	AY	365	0	185	29	0
23	CW	1619	0	822	109	0
23	CY	365	0	185	37	0
24	AX	255	0	129	49	0
24	CX	210	0	109	23	0
25	BA	60527	0	30515	1623	1
25	DA	60827	0	30663	1373	0
26	BB	2551	0	1295	57	1
26	DB	2551	0	1295	55	0
27	BC	1142	0	865	78	0
27	DC	1142	0	865	70	0
28	BD	2105	0	2182	310	0
28	DD	2105	0	2182	277	0
29	BE	1564	0	1629	216	0
29	DE	1564	0	1629	206	0
30	BF	1624	0	1677	246	0
30	DF	1585	0	1632	188	0
31	BG	1474	0	1535	264	0
31	DG	1474	0	1535	209	0
32	BH	1223	0	1282	136	1
32	DH	1290	0	1364	238	0
33	BI	1131	0	1218	152	0
33	DI	1136	0	1223	229	0
34	BN	1105	0	1180	188	0
34	DN	1105	0	1180	140	0
35	BO	933	0	996	117	0
35	DO	933	0	996	90	0
36	BP	1145	0	1228	279	0
36	DP	1145	0	1228	283	3
37	BQ	1122	0	1179	129	0
37	DQ	1122	0	1179	123	0
38	BR	960	0	1021	146	0
38	DR	968	0	1033	109	0
39	BS	771	0	832	127	0
39	DS	882	0	943	149	0
40	BT	1142	0	1202	240	0
40	DT	1142	0	1202	269	0
41	BU	964	0	1022	160	0
41	DU	958	0	1014	198	0
42	BV	779	0	852	135	0
42	DV	779	0	852	150	3
43	BW	896	0	953	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DW	896	0	953	89	0
44	BX	726	0	778	64	0
44	DX	726	0	778	67	0
45	BY	776	0	870	172	0
45	DY	785	0	878	176	0
46	BZ	1404	0	1432	148	0
46	DZ	1404	0	1432	214	0
47	B0	662	0	688	60	0
47	D0	662	0	688	60	0
48	B1	732	0	808	78	0
48	D1	732	0	808	66	0
49	B2	598	0	653	64	0
49	D2	598	0	653	53	0
50	B3	468	0	523	40	3
50	D3	468	0	523	50	0
51	B4	226	0	229	39	0
51	D4	298	0	312	43	0
52	B5	459	0	480	50	0
52	D5	459	0	480	53	3
53	B6	381	0	391	51	0
53	D6	381	0	391	99	0
54	B7	419	0	467	35	0
54	D7	419	0	467	33	0
55	B8	508	0	576	115	0
55	D8	508	0	576	85	0
56	B9	299	0	326	13	0
56	D9	299	0	326	14	0
57	AA	110	0	0	0	0
57	AE	1	0	0	0	0
57	AV	5	0	0	0	0
57	AX	1	0	0	0	0
57	B5	1	0	0	0	0
57	B7	1	0	0	0	0
57	BA	323	0	0	0	0
57	BB	5	0	0	0	0
57	BD	2	0	0	0	0
57	BE	3	0	0	0	0
57	BF	1	0	0	0	0
57	BN	1	0	0	0	0
57	BO	1	0	0	0	0
57	BP	1	0	0	0	0
57	BU	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	CA	141	0	0	0	0
57	CE	2	0	0	0	0
57	CV	5	0	0	0	0
57	CW	1	0	0	0	0
57	CX	1	0	0	0	0
57	CY	1	0	0	0	0
57	D0	2	0	0	0	0
57	D1	2	0	0	0	0
57	D2	1	0	0	0	0
57	D5	2	0	0	0	0
57	D8	1	0	0	0	0
57	DA	397	0	0	0	0
57	DB	5	0	0	0	0
57	DD	3	0	0	0	0
57	DE	2	0	0	0	0
57	DF	1	0	0	0	0
57	DP	3	0	0	0	0
57	DQ	1	0	0	0	0
57	DU	3	0	0	0	0
57	DW	1	0	0	0	0
57	DX	1	0	0	0	0
58	AA	42	0	45	3	0
58	CA	42	0	45	2	0
59	AD	1	0	0	0	0
59	AN	1	0	0	1	0
59	CD	1	0	0	0	0
59	CN	1	0	0	3	0
All	All	293977	0	199058	16442	8

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 34.

The worst 5 of 16442 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
39:BS:34:HIS:CE1	39:BS:54:LEU:HB2	1.32	1.58
42:DV:1:MET:SD	42:DV:1:MET:CG	2.01	1.47
40:BT:28:VAL:CG1	40:BT:46:GLU:HA	1.42	1.44
1:CA:748:C:H1'	1:CA:749:C:C5	1.53	1.44
34:BN:62:VAL:HG22	34:BN:66:LYS:CD	1.49	1.42

The worst 5 of 8 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
50:B3:1:MET:N	36:DP:122:PRO:CG[3.455]	1.46	0.74
50:B3:1:MET:N	36:DP:122:PRO:CD[3.455]	1.64	0.56
42:DV:50:PRO:CG	52:D5:58:LEU:O[4.445]	1.80	0.40
42:DV:48:GLY:O	52:D5:58:LEU:CD1[4.445]	1.84	0.36
25:BA:1593:G:O2'	26:BB:54:G:OP1[1.655]	2.09	0.11

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	159 (68%)	53 (23%)	21 (9%)	1	18
2	CB	233/256 (91%)	158 (68%)	45 (19%)	30 (13%)	0	10
3	AC	205/239 (86%)	129 (63%)	54 (26%)	22 (11%)	1	13
3	CC	205/239 (86%)	135 (66%)	52 (25%)	18 (9%)	1	19
4	AD	206/209 (99%)	142 (69%)	43 (21%)	21 (10%)	1	15
4	CD	206/209 (99%)	141 (68%)	47 (23%)	18 (9%)	1	19
5	AE	149/162 (92%)	117 (78%)	20 (13%)	12 (8%)	1	21
5	CE	149/162 (92%)	113 (76%)	22 (15%)	14 (9%)	1	17
6	AF	99/101 (98%)	63 (64%)	29 (29%)	7 (7%)	2	26
6	CF	99/101 (98%)	80 (81%)	14 (14%)	5 (5%)	3	36
7	AG	153/156 (98%)	116 (76%)	26 (17%)	11 (7%)	2	25
7	CG	153/156 (98%)	117 (76%)	29 (19%)	7 (5%)	4	40
8	AH	136/138 (99%)	96 (71%)	35 (26%)	5 (4%)	5	48
8	CH	136/138 (99%)	102 (75%)	28 (21%)	6 (4%)	4	42
9	AI	125/128 (98%)	84 (67%)	32 (26%)	9 (7%)	2	25
9	CI	125/128 (98%)	87 (70%)	23 (18%)	15 (12%)	1	11
10	AJ	97/105 (92%)	59 (61%)	31 (32%)	7 (7%)	2	25
10	CJ	97/105 (92%)	60 (62%)	25 (26%)	12 (12%)	1	11
11	AK	117/129 (91%)	92 (79%)	19 (16%)	6 (5%)	3	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	CK	117/129 (91%)	92 (79%)	23 (20%)	2 (2%)	14	67
12	AL	123/132 (93%)	78 (63%)	25 (20%)	20 (16%)	0	5
12	CL	123/132 (93%)	91 (74%)	20 (16%)	12 (10%)	1	16
13	AM	123/126 (98%)	82 (67%)	23 (19%)	18 (15%)	0	6
13	CM	123/126 (98%)	78 (63%)	22 (18%)	23 (19%)	0	3
14	AN	58/61 (95%)	40 (69%)	11 (19%)	7 (12%)	1	11
14	CN	58/61 (95%)	37 (64%)	14 (24%)	7 (12%)	1	11
15	AO	86/89 (97%)	65 (76%)	20 (23%)	1 (1%)	19	75
15	CO	86/89 (97%)	55 (64%)	25 (29%)	6 (7%)	2	26
16	AP	82/88 (93%)	53 (65%)	25 (30%)	4 (5%)	3	38
16	CP	82/88 (93%)	66 (80%)	13 (16%)	3 (4%)	5	48
17	AQ	98/105 (93%)	79 (81%)	13 (13%)	6 (6%)	2	30
17	CQ	98/105 (93%)	77 (79%)	15 (15%)	6 (6%)	2	30
18	AR	68/88 (77%)	49 (72%)	12 (18%)	7 (10%)	1	14
18	CR	68/88 (77%)	49 (72%)	11 (16%)	8 (12%)	1	12
19	AS	77/93 (83%)	56 (73%)	15 (20%)	6 (8%)	1	22
19	CS	77/93 (83%)	47 (61%)	17 (22%)	13 (17%)	0	4
20	AT	97/106 (92%)	68 (70%)	22 (23%)	7 (7%)	2	25
20	CT	97/106 (92%)	67 (69%)	18 (19%)	12 (12%)	1	11
21	AU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	4
21	CU	23/27 (85%)	18 (78%)	3 (13%)	2 (9%)	1	19
27	BC	183/229 (80%)	85 (46%)	52 (28%)	46 (25%)	0	1
27	DC	183/229 (80%)	87 (48%)	45 (25%)	51 (28%)	0	0
28	BD	270/276 (98%)	200 (74%)	38 (14%)	32 (12%)	1	12
28	DD	270/276 (98%)	202 (75%)	44 (16%)	24 (9%)	1	18
29	BE	203/206 (98%)	145 (71%)	36 (18%)	22 (11%)	1	13
29	DE	203/206 (98%)	134 (66%)	36 (18%)	33 (16%)	0	5
30	BF	206/210 (98%)	142 (69%)	44 (21%)	20 (10%)	1	16
30	DF	200/210 (95%)	160 (80%)	29 (14%)	11 (6%)	3	34
31	BG	179/182 (98%)	121 (68%)	36 (20%)	22 (12%)	1	11
31	DG	179/182 (98%)	124 (69%)	30 (17%)	25 (14%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BH	158/180 (88%)	96 (61%)	37 (23%)	25 (16%)	0	5
32	DH	166/180 (92%)	96 (58%)	42 (25%)	28 (17%)	0	4
33	BI	143/148 (97%)	101 (71%)	26 (18%)	16 (11%)	1	13
33	DI	144/148 (97%)	78 (54%)	39 (27%)	27 (19%)	0	3
34	BN	137/140 (98%)	91 (66%)	24 (18%)	22 (16%)	0	5
34	DN	137/140 (98%)	86 (63%)	39 (28%)	12 (9%)	1	19
35	BO	120/122 (98%)	95 (79%)	17 (14%)	8 (7%)	2	28
35	DO	120/122 (98%)	97 (81%)	18 (15%)	5 (4%)	4	43
36	BP	148/150 (99%)	86 (58%)	26 (18%)	36 (24%)	0	1
36	DP	148/150 (99%)	86 (58%)	23 (16%)	39 (26%)	0	1
37	BQ	139/141 (99%)	104 (75%)	24 (17%)	11 (8%)	1	22
37	DQ	139/141 (99%)	109 (78%)	18 (13%)	12 (9%)	1	20
38	BR	115/118 (98%)	78 (68%)	25 (22%)	12 (10%)	1	14
38	DR	116/118 (98%)	86 (74%)	20 (17%)	10 (9%)	1	20
39	BS	97/112 (87%)	53 (55%)	16 (16%)	28 (29%)	0	0
39	DS	109/112 (97%)	71 (65%)	21 (19%)	17 (16%)	0	5
40	BT	136/146 (93%)	90 (66%)	28 (21%)	18 (13%)	0	9
40	DT	136/146 (93%)	95 (70%)	19 (14%)	22 (16%)	0	5
41	BU	115/118 (98%)	73 (64%)	30 (26%)	12 (10%)	1	14
41	DU	115/118 (98%)	75 (65%)	30 (26%)	10 (9%)	1	19
42	BV	99/101 (98%)	75 (76%)	9 (9%)	15 (15%)	0	5
42	DV	99/101 (98%)	80 (81%)	9 (9%)	10 (10%)	1	15
43	BW	111/113 (98%)	81 (73%)	22 (20%)	8 (7%)	2	25
43	DW	111/113 (98%)	82 (74%)	19 (17%)	10 (9%)	1	18
44	BX	91/96 (95%)	69 (76%)	16 (18%)	6 (7%)	2	28
44	DX	91/96 (95%)	76 (84%)	11 (12%)	4 (4%)	4	42
45	BY	99/110 (90%)	50 (50%)	22 (22%)	27 (27%)	0	1
45	DY	100/110 (91%)	64 (64%)	11 (11%)	25 (25%)	0	1
46	BZ	175/206 (85%)	114 (65%)	40 (23%)	21 (12%)	1	11
46	DZ	175/206 (85%)	101 (58%)	46 (26%)	28 (16%)	0	5
47	B0	82/85 (96%)	64 (78%)	13 (16%)	5 (6%)	2	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	D0	82/85 (96%)	67 (82%)	8 (10%)	7 (8%)	1	20
48	B1	92/98 (94%)	68 (74%)	13 (14%)	11 (12%)	1	11
48	D1	92/98 (94%)	69 (75%)	12 (13%)	11 (12%)	1	11
49	B2	69/72 (96%)	49 (71%)	15 (22%)	5 (7%)	2	25
49	D2	69/72 (96%)	57 (83%)	5 (7%)	7 (10%)	1	15
50	B3	58/60 (97%)	48 (83%)	3 (5%)	7 (12%)	1	11
50	D3	58/60 (97%)	46 (79%)	7 (12%)	5 (9%)	1	20
51	B4	29/71 (41%)	17 (59%)	8 (28%)	4 (14%)	0	8
51	D4	38/71 (54%)	21 (55%)	12 (32%)	5 (13%)	0	9
52	B5	57/60 (95%)	46 (81%)	6 (10%)	5 (9%)	1	19
52	D5	57/60 (95%)	46 (81%)	5 (9%)	6 (10%)	1	14
53	B6	43/54 (80%)	17 (40%)	14 (33%)	12 (28%)	0	0
53	D6	43/54 (80%)	18 (42%)	15 (35%)	10 (23%)	0	1
54	B7	47/49 (96%)	38 (81%)	5 (11%)	4 (8%)	1	20
54	D7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	11	62
55	B8	62/65 (95%)	42 (68%)	14 (23%)	6 (10%)	1	16
55	D8	62/65 (95%)	41 (66%)	14 (23%)	7 (11%)	1	13
56	B9	34/37 (92%)	23 (68%)	10 (29%)	1 (3%)	7	54
56	D9	34/37 (92%)	27 (79%)	6 (18%)	1 (3%)	7	54
All	All	11730/12586 (93%)	8097 (69%)	2283 (20%)	1350 (12%)	1	12

5 of 1350 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	195	ASP
2	AB	238	LEU
3	AC	18	TRP
3	AC	20	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain

conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	161 (80%)	41 (20%)	2	11
2	CB	202/220 (92%)	155 (77%)	47 (23%)	1	7
3	AC	160/188 (85%)	127 (79%)	33 (21%)	2	10
3	CC	160/188 (85%)	130 (81%)	30 (19%)	2	13
4	AD	180/181 (99%)	149 (83%)	31 (17%)	3	18
4	CD	180/181 (99%)	151 (84%)	29 (16%)	3	22
5	AE	115/123 (94%)	97 (84%)	18 (16%)	4	23
5	CE	115/123 (94%)	87 (76%)	28 (24%)	1	6
6	AF	90/90 (100%)	76 (84%)	14 (16%)	4	23
6	CF	90/90 (100%)	79 (88%)	11 (12%)	7	35
7	AG	126/127 (99%)	103 (82%)	23 (18%)	2	14
7	CG	126/127 (99%)	106 (84%)	20 (16%)	4	22
8	AH	119/119 (100%)	101 (85%)	18 (15%)	4	25
8	CH	119/119 (100%)	87 (73%)	32 (27%)	1	5
9	AI	98/99 (99%)	77 (79%)	21 (21%)	1	9
9	CI	98/99 (99%)	72 (74%)	26 (26%)	1	5
10	AJ	88/92 (96%)	66 (75%)	22 (25%)	1	6
10	CJ	88/92 (96%)	66 (75%)	22 (25%)	1	6
11	AK	90/99 (91%)	74 (82%)	16 (18%)	2	16
11	CK	90/99 (91%)	72 (80%)	18 (20%)	2	11
12	AL	104/109 (95%)	85 (82%)	19 (18%)	2	14
12	CL	104/109 (95%)	84 (81%)	20 (19%)	2	12
13	AM	99/101 (98%)	82 (83%)	17 (17%)	3	18
13	CM	100/101 (99%)	83 (83%)	17 (17%)	3	18
14	AN	49/50 (98%)	37 (76%)	12 (24%)	1	6
14	CN	49/50 (98%)	38 (78%)	11 (22%)	1	8
15	AO	79/80 (99%)	64 (81%)	15 (19%)	2	13
15	CO	79/80 (99%)	66 (84%)	13 (16%)	3	20
16	AP	72/74 (97%)	58 (81%)	14 (19%)	2	12
16	CP	72/74 (97%)	58 (81%)	14 (19%)	2	12
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	15	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	CQ	94/97 (97%)	82 (87%)	12 (13%)	6	33
18	AR	61/77 (79%)	51 (84%)	10 (16%)	3	21
18	CR	61/77 (79%)	50 (82%)	11 (18%)	2	15
19	AS	69/80 (86%)	51 (74%)	18 (26%)	1	5
19	CS	69/80 (86%)	49 (71%)	20 (29%)	0	4
20	AT	76/82 (93%)	56 (74%)	20 (26%)	1	5
20	CT	76/82 (93%)	53 (70%)	23 (30%)	0	4
21	AU	19/22 (86%)	18 (95%)	1 (5%)	32	78
21	CU	19/22 (86%)	14 (74%)	5 (26%)	1	5
27	BC	61/181 (34%)	49 (80%)	12 (20%)	2	11
27	DC	61/181 (34%)	53 (87%)	8 (13%)	6	32
28	BD	213/218 (98%)	164 (77%)	49 (23%)	1	7
28	DD	213/218 (98%)	178 (84%)	35 (16%)	3	21
29	BE	165/166 (99%)	125 (76%)	40 (24%)	1	6
29	DE	165/166 (99%)	141 (86%)	24 (14%)	5	27
30	BF	165/166 (99%)	127 (77%)	38 (23%)	1	7
30	DF	161/166 (97%)	136 (84%)	25 (16%)	4	23
31	BG	155/156 (99%)	118 (76%)	37 (24%)	1	6
31	DG	155/156 (99%)	135 (87%)	20 (13%)	6	33
32	BH	132/148 (89%)	114 (86%)	18 (14%)	5	30
32	DH	140/148 (95%)	114 (81%)	26 (19%)	2	13
33	BI	122/124 (98%)	95 (78%)	27 (22%)	1	8
33	DI	122/124 (98%)	92 (75%)	30 (25%)	1	6
34	BN	117/119 (98%)	88 (75%)	29 (25%)	1	6
34	DN	117/119 (98%)	96 (82%)	21 (18%)	2	15
35	BO	100/100 (100%)	77 (77%)	23 (23%)	1	7
35	DO	100/100 (100%)	90 (90%)	10 (10%)	11	48
36	BP	116/116 (100%)	86 (74%)	30 (26%)	1	5
36	DP	116/116 (100%)	89 (77%)	27 (23%)	1	7
37	BQ	111/111 (100%)	81 (73%)	30 (27%)	1	5
37	DQ	111/111 (100%)	92 (83%)	19 (17%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BR	100/101 (99%)	68 (68%)	32 (32%)	0	3
38	DR	101/101 (100%)	86 (85%)	15 (15%)	4	26
39	BS	77/88 (88%)	56 (73%)	21 (27%)	0	4
39	DS	87/88 (99%)	75 (86%)	12 (14%)	5	29
40	BT	120/127 (94%)	90 (75%)	30 (25%)	1	6
40	DT	120/127 (94%)	91 (76%)	29 (24%)	1	6
41	BU	93/94 (99%)	70 (75%)	23 (25%)	1	6
41	DU	92/94 (98%)	80 (87%)	12 (13%)	6	33
42	BV	82/82 (100%)	55 (67%)	27 (33%)	0	3
42	DV	82/82 (100%)	64 (78%)	18 (22%)	1	8
43	BW	91/92 (99%)	69 (76%)	22 (24%)	1	6
43	DW	91/92 (99%)	83 (91%)	8 (9%)	14	57
44	BX	74/78 (95%)	58 (78%)	16 (22%)	1	9
44	DX	74/78 (95%)	61 (82%)	13 (18%)	3	16
45	BY	84/91 (92%)	67 (80%)	17 (20%)	2	11
45	DY	85/91 (93%)	66 (78%)	19 (22%)	1	8
46	BZ	155/179 (87%)	124 (80%)	31 (20%)	2	11
46	DZ	155/179 (87%)	136 (88%)	19 (12%)	7	35
47	B0	66/67 (98%)	57 (86%)	9 (14%)	5	30
47	D0	66/67 (98%)	57 (86%)	9 (14%)	5	30
48	B1	78/83 (94%)	61 (78%)	17 (22%)	1	9
48	D1	78/83 (94%)	61 (78%)	17 (22%)	1	9
49	B2	66/67 (98%)	53 (80%)	13 (20%)	2	11
49	D2	66/67 (98%)	53 (80%)	13 (20%)	2	11
50	B3	51/52 (98%)	40 (78%)	11 (22%)	1	9
50	D3	51/52 (98%)	49 (96%)	2 (4%)	43	85
51	B4	27/63 (43%)	17 (63%)	10 (37%)	0	1
51	D4	35/63 (56%)	31 (89%)	4 (11%)	8	40
52	B5	51/52 (98%)	42 (82%)	9 (18%)	3	16
52	D5	51/52 (98%)	43 (84%)	8 (16%)	4	23
53	B6	43/52 (83%)	31 (72%)	12 (28%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	D6	43/52 (83%)	33 (77%)	10 (23%)	1	7
54	B7	41/42 (98%)	35 (85%)	6 (15%)	5	27
54	D7	41/42 (98%)	37 (90%)	4 (10%)	12	49
55	B8	53/55 (96%)	38 (72%)	15 (28%)	0	4
55	D8	53/55 (96%)	41 (77%)	12 (23%)	1	8
56	B9	33/34 (97%)	29 (88%)	4 (12%)	7	36
56	D9	33/34 (97%)	29 (88%)	4 (12%)	7	36
All	All	9688/10428 (93%)	7777 (80%)	1911 (20%)	2	11

5 of 1911 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	BX	43	VAL
2	CB	196	LEU
42	DV	91	TYR
45	BY	89	PHE
50	B3	53	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
2	CB	204	ASN
12	CL	9	GLN
48	D1	45	ASN
5	CE	78	HIS
9	CI	38	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	366 (24%)	109 (7%)
1	CA	1503/1522 (98%)	359 (23%)	115 (7%)
22	AV	76/77 (98%)	26 (34%)	3 (3%)
22	CV	76/77 (98%)	30 (39%)	4 (5%)
23	AW	75/76 (98%)	22 (29%)	0
23	AY	16/76 (21%)	5 (31%)	0
23	CW	75/76 (98%)	26 (34%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	CY	16/76 (21%)	8 (50%)	0
24	AX	11/24 (45%)	4 (36%)	0
24	CX	9/24 (37%)	4 (44%)	1 (11%)
25	BA	2804/2915 (96%)	803 (28%)	260 (9%)
25	DA	2818/2915 (96%)	804 (28%)	264 (9%)
26	BB	118/122 (96%)	25 (21%)	5 (4%)
26	DB	118/122 (96%)	24 (20%)	7 (5%)
All	All	9218/9624 (95%)	2506 (27%)	768 (8%)

5 of 2506 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	10	A
1	AA	13	U

5 of 768 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	2602	A
1	CA	575	G
25	DA	2238	G
25	BA	2750	A
1	CA	129(A)	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1039 ligands modelled in this entry, 1037 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	PAR	AA	7111	-	45,45,45	1.44	8 (17%)	67,67,67	1.19	5 (7%)
58	PAR	CA	1741	-	45,45,45	1.44	8 (17%)	67,67,67	1.19	6 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PAR	AA	7111	-	-	0/18/94/94	0/4/4/4
58	PAR	CA	1741	-	-	0/18/94/94	0/4/4/4

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AA	7111	PAR	O54-C14	3.93	1.51	1.41
58	CA	1741	PAR	O54-C14	3.90	1.51	1.41
58	CA	1741	PAR	C31-C21	2.98	1.57	1.53
58	AA	7111	PAR	C31-C21	2.93	1.57	1.53
58	AA	7111	PAR	C24-N24	2.70	1.51	1.47

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	CA	1741	PAR	C14-O54-C54	3.25	120.01	113.73
58	AA	7111	PAR	C14-O54-C54	3.24	120.01	113.73
58	AA	7111	PAR	O54-C54-C64	3.17	112.00	105.97
58	CA	1741	PAR	O54-C54-C64	3.16	111.99	105.97
58	AA	7111	PAR	O33-C14-C24	2.99	113.99	108.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	BA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	1453:U	O3'	1455:G	P	1.97

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	0.12	41 (2%)	52	25	31, 78, 168, 331	0
1	CA	1504/1522 (98%)	0.14	52 (3%)	42	20	24, 68, 165, 363	0
2	AB	235/256 (91%)	0.16	6 (2%)	53	25	67, 121, 201, 279	0
2	CB	235/256 (91%)	0.16	8 (3%)	43	20	44, 109, 202, 287	0
3	AC	207/239 (86%)	0.13	2 (0%)	79	48	44, 104, 173, 240	0
3	CC	207/239 (86%)	0.06	1 (0%)	88	65	38, 90, 151, 227	0
4	AD	208/209 (99%)	0.01	1 (0%)	88	65	37, 89, 153, 217	0
4	CD	208/209 (99%)	-0.00	1 (0%)	88	65	30, 77, 129, 209	0
5	AE	151/162 (93%)	0.04	1 (0%)	84	56	44, 87, 151, 240	0
5	CE	151/162 (93%)	0.03	1 (0%)	84	56	22, 71, 131, 266	0
6	AF	101/101 (100%)	0.06	0	100	100	29, 74, 120, 178	0
6	CF	101/101 (100%)	-0.00	0	100	100	25, 68, 134, 192	0
7	AG	155/156 (99%)	0.12	6 (3%)	37	17	50, 93, 149, 256	0
7	CG	155/156 (99%)	0.12	5 (3%)	45	21	32, 87, 151, 269	0
8	AH	138/138 (100%)	-0.00	0	100	100	41, 85, 129, 183	0
8	CH	138/138 (100%)	-0.05	1 (0%)	84	56	38, 75, 123, 181	0
9	AI	127/128 (99%)	0.27	2 (1%)	68	36	55, 113, 161, 319	0
9	CI	127/128 (99%)	0.19	2 (1%)	68	36	45, 97, 170, 245	0
10	AJ	99/105 (94%)	0.52	3 (3%)	48	23	58, 124, 197, 302	0
10	CJ	99/105 (94%)	0.50	5 (5%)	27	12	38, 115, 191, 204	0
11	AK	119/129 (92%)	0.12	4 (3%)	43	20	41, 77, 147, 249	0
11	CK	119/129 (92%)	0.19	4 (3%)	43	20	29, 73, 139, 188	0
12	AL	125/132 (94%)	0.11	3 (2%)	56	27	31, 64, 129, 300	0
12	CL	125/132 (94%)	-0.01	3 (2%)	56	27	9, 47, 127, 252	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	0.27	6 (4%) 29 13	29, 94, 148, 314	0
13	CM	125/126 (99%)	0.31	6 (4%) 29 13	39, 87, 174, 274	0
14	AN	60/61 (98%)	0.21	1 (1%) 67 35	53, 92, 138, 207	0
14	CN	60/61 (98%)	0.16	1 (1%) 67 35	34, 71, 111, 194	0
15	AO	88/89 (98%)	0.02	0 100 100	35, 80, 132, 142	0
15	CO	88/89 (98%)	-0.02	1 (1%) 77 45	23, 69, 122, 147	0
16	AP	84/88 (95%)	-0.11	0 100 100	48, 74, 122, 182	0
16	CP	84/88 (95%)	-0.01	0 100 100	44, 76, 139, 200	0
17	AQ	100/105 (95%)	0.09	0 100 100	50, 91, 141, 174	0
17	CQ	100/105 (95%)	0.11	1 (1%) 79 48	38, 87, 144, 192	0
18	AR	70/88 (79%)	0.11	3 (4%) 34 15	35, 77, 126, 183	0
18	CR	70/88 (79%)	-0.03	1 (1%) 72 39	36, 70, 122, 205	0
19	AS	79/93 (84%)	0.36	0 100 100	46, 104, 202, 268	0
19	CS	79/93 (84%)	0.35	1 (1%) 74 41	27, 82, 153, 206	0
20	AT	99/106 (93%)	0.31	4 (4%) 36 17	42, 90, 173, 211	0
20	CT	99/106 (93%)	0.36	3 (3%) 48 23	40, 97, 192, 295	0
21	AU	25/27 (92%)	1.04	5 (20%) 2 2	36, 92, 165, 229	0
21	CU	25/27 (92%)	0.46	1 (4%) 36 17	50, 78, 107, 150	0
22	AV	77/77 (100%)	0.05	0 100 100	45, 82, 163, 276	0
22	CV	77/77 (100%)	0.15	3 (3%) 37 17	32, 72, 133, 253	0
23	AW	76/76 (100%)	1.16	14 (18%) 2 2	48, 175, 249, 317	0
23	AY	17/76 (22%)	0.34	0 100 100	64, 94, 167, 176	0
23	CW	76/76 (100%)	1.44	20 (26%) 1 2	34, 184, 271, 295	0
23	CY	17/76 (22%)	0.54	0 100 100	44, 75, 149, 186	0
24	AX	12/24 (50%)	0.88	3 (25%) 1 2	49, 74, 217, 234	0
24	CX	10/24 (41%)	0.65	1 (10%) 8 5	42, 58, 144, 213	0
25	BA	2810/2915 (96%)	0.11	93 (3%) 44 21	17, 58, 187, 375	0
25	DA	2824/2915 (96%)	0.04	94 (3%) 44 21	6, 42, 178, 370	0
26	BB	119/122 (97%)	0.09	0 100 100	59, 94, 132, 182	0
26	DB	119/122 (97%)	0.08	2 (1%) 67 35	38, 68, 113, 174	0
27	BC	191/229 (83%)	1.68	66 (34%) 1 1	89, 200, 319, 378	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	DC	191/229 (83%)	1.98	83 (43%) 1 1	64, 208, 290, 334	0
28	BD	272/276 (98%)	-0.08	0 100 100	9, 45, 89, 166	0
28	DD	272/276 (98%)	-0.15	0 100 100	3, 33, 80, 197	0
29	BE	205/206 (99%)	0.04	5 (2%) 56 27	17, 66, 128, 289	0
29	DE	205/206 (99%)	0.04	4 (1%) 62 31	11, 55, 160, 338	0
30	BF	208/210 (99%)	-0.04	4 (1%) 64 32	14, 64, 164, 286	0
30	DF	202/210 (96%)	-0.03	2 (0%) 79 48	5, 51, 127, 208	0
31	BG	181/182 (99%)	0.08	5 (2%) 50 24	40, 95, 175, 268	0
31	DG	181/182 (99%)	0.10	3 (1%) 67 35	25, 76, 143, 219	0
32	BH	160/180 (88%)	0.92	29 (18%) 2 2	85, 179, 331, 429	0
32	DH	168/180 (93%)	0.25	0 100 100	29, 81, 155, 234	0
33	BI	145/148 (97%)	0.13	3 (2%) 60 30	33, 96, 156, 185	0
33	DI	146/148 (98%)	0.16	0 100 100	15, 104, 166, 207	0
34	BN	139/140 (99%)	0.02	1 (0%) 84 56	36, 79, 147, 305	0
34	DN	139/140 (99%)	-0.03	0 100 100	7, 61, 137, 185	0
35	BO	122/122 (100%)	-0.16	0 100 100	32, 65, 97, 124	0
35	DO	122/122 (100%)	-0.25	0 100 100	10, 41, 84, 112	0
36	BP	150/150 (100%)	0.48	6 (4%) 36 17	27, 87, 179, 250	0
36	DP	150/150 (100%)	0.29	2 (1%) 74 41	23, 71, 151, 264	0
37	BQ	141/141 (100%)	0.09	2 (1%) 72 39	36, 74, 126, 421	0
37	DQ	141/141 (100%)	-0.07	0 100 100	12, 52, 108, 281	0
38	BR	117/118 (99%)	-0.08	0 100 100	21, 57, 107, 148	0
38	DR	118/118 (100%)	-0.12	0 100 100	15, 50, 92, 126	0
39	BS	99/112 (88%)	0.08	0 100 100	38, 100, 171, 347	0
39	DS	111/112 (99%)	0.13	2 (1%) 65 34	33, 73, 147, 197	0
40	BT	138/146 (94%)	0.26	6 (4%) 34 15	29, 80, 225, 351	0
40	DT	138/146 (94%)	0.22	7 (5%) 27 12	20, 71, 212, 304	0
41	BU	117/118 (99%)	-0.09	1 (0%) 81 51	29, 64, 131, 281	0
41	DU	117/118 (99%)	-0.16	1 (0%) 81 51	17, 52, 114, 180	0
42	BV	101/101 (100%)	0.00	0 100 100	23, 90, 149, 344	0
42	DV	101/101 (100%)	0.13	1 (0%) 79 48	9, 70, 131, 303	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BW	113/113 (100%)	0.06	2 (1%) 65 34	19, 49, 113, 319	0
43	DW	113/113 (100%)	-0.02	0 100 100	14, 42, 128, 204	0
44	BX	93/96 (96%)	-0.02	0 100 100	30, 63, 99, 149	0
44	DX	93/96 (96%)	-0.03	0 100 100	12, 42, 87, 144	0
45	BY	101/110 (91%)	0.94	18 (17%) 2 2	42, 92, 253, 363	0
45	DY	102/110 (92%)	0.30	3 (2%) 49 24	28, 82, 182, 226	0
46	BZ	177/206 (85%)	0.55	14 (7%) 13 7	45, 125, 202, 316	0
46	DZ	177/206 (85%)	0.66	14 (7%) 13 7	29, 116, 254, 322	0
47	B0	84/85 (98%)	0.21	4 (4%) 29 13	31, 69, 170, 242	0
47	D0	84/85 (98%)	0.16	4 (4%) 29 13	18, 52, 136, 286	0
48	B1	94/98 (95%)	0.11	1 (1%) 77 45	17, 53, 113, 219	0
48	D1	94/98 (95%)	-0.00	0 100 100	7, 44, 122, 237	0
49	B2	71/72 (98%)	0.08	2 (2%) 50 24	35, 77, 128, 195	0
49	D2	71/72 (98%)	0.06	0 100 100	14, 54, 137, 267	0
50	B3	60/60 (100%)	0.24	2 (3%) 44 21	35, 75, 125, 382	0
50	D3	60/60 (100%)	0.05	1 (1%) 67 35	20, 65, 142, 236	0
51	B4	31/71 (43%)	0.07	0 100 100	67, 121, 152, 204	0
51	D4	40/71 (56%)	0.27	2 (5%) 28 12	55, 116, 173, 266	0
52	B5	59/60 (98%)	0.37	5 (8%) 11 6	17, 72, 180, 340	0
52	D5	59/60 (98%)	0.34	3 (5%) 27 12	12, 63, 214, 299	0
53	B6	45/54 (83%)	1.19	8 (17%) 2 2	44, 138, 207, 343	0
53	D6	45/54 (83%)	1.56	13 (28%) 1 1	59, 139, 235, 285	0
54	B7	49/49 (100%)	-0.05	1 (2%) 62 31	11, 41, 123, 149	0
54	D7	49/49 (100%)	-0.21	0 100 100	1, 23, 101, 204	0
55	B8	64/65 (98%)	0.21	1 (1%) 68 36	20, 60, 129, 325	0
55	D8	64/65 (98%)	-0.08	0 100 100	12, 51, 115, 172	0
56	B9	36/37 (97%)	3.71	29 (80%) 0 0	120, 197, 269, 389	0
56	D9	36/37 (97%)	3.33	31 (86%) 0 0	115, 172, 217, 282	0
All	All	21184/22210 (95%)	0.17	807 (3%) 38 18	1, 71, 192, 429	0

The worst 5 of 807 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	DA	2802	G	15.2
25	BA	2802	G	13.1
1	AA	89	C	12.8
56	B9	14	CYS	12.7
1	AA	81	U	12.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
57	MG	BA	3018	1/1	0.17	-	37,37,37,37	0
57	MG	BA	3293	1/1	0.23	-	1,1,1,1	0
57	MG	BA	3074	1/1	0.61	-	34,34,34,34	0
57	MG	BA	3242	1/1	0.57	-	44,44,44,44	0
57	MG	BA	3275	1/1	0.27	-	1,1,1,1	1
57	MG	DA	9354	1/1	0.48	-	2,2,2,2	0
57	MG	AA	7037	1/1	0.34	-	7,7,7,7	0
57	MG	BA	3132	1/1	0.28	-	51,51,51,51	0
57	MG	DA	9391	1/1	0.16	-	1,1,1,1	0
57	MG	AA	7063	1/1	0.27	-	31,31,31,31	0
57	MG	AA	7020	1/1	0.36	-	33,33,33,33	0
57	MG	DA	9649	1/1	0.46	-	1,1,1,1	0
57	MG	DA	9673	1/1	0.41	-	8,8,8,8	0
59	ZN	CD	301	1/1	0.32	-	44,44,44,44	0
57	MG	DA	9680	1/1	0.41	-	24,24,24,24	0
57	MG	CA	1614	1/1	1.21	-	38,38,38,38	0
57	MG	CA	1657	1/1	0.28	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9307	1/1	0.35	-	12,12,12,12	0
57	MG	DA	9528	1/1	0.37	-	6,6,6,6	0
57	MG	BA	3055	1/1	0.21	-	11,11,11,11	0
57	MG	BA	3180	1/1	0.62	-	2,2,2,2	0
57	MG	CA	1716	1/1	0.48	-	26,26,26,26	0
57	MG	BA	3031	1/1	0.23	-	44,44,44,44	0
57	MG	BA	3321	1/1	0.37	-	35,35,35,35	0
57	MG	BN	201	1/1	0.31	-	125,125,125,125	1
57	MG	AA	7080	1/1	0.41	-	8,8,8,8	1
57	MG	BA	3114	1/1	0.33	-	41,41,41,41	0
57	MG	D8	101	1/1	0.22	-	3,3,3,3	0
57	MG	DA	9606	1/1	0.94	-	4,4,4,4	0
57	MG	BA	3310	1/1	0.39	-	35,35,35,35	0
57	MG	BA	3305	1/1	0.24	-	24,24,24,24	0
57	MG	DA	9542	1/1	0.34	-	6,6,6,6	0
57	MG	BA	3170	1/1	0.78	-	1,1,1,1	0
57	MG	DA	9552	1/1	0.57	-	58,58,58,58	0
57	MG	AA	7106	1/1	0.25	-	12,12,12,12	0
57	MG	BA	3049	1/1	0.53	-	30,30,30,30	0
57	MG	BA	3230	1/1	0.61	-	22,22,22,22	0
57	MG	DA	9671	1/1	0.20	-	45,45,45,45	0
57	MG	DA	9311	1/1	0.46	-	29,29,29,29	0
57	MG	DA	9524	1/1	0.36	-	2,2,2,2	0
57	MG	BA	3169	1/1	0.52	-	3,3,3,3	0
57	MG	DA	9407	1/1	0.23	-	2,2,2,2	0
57	MG	BA	3195	1/1	0.30	-	3,3,3,3	0
57	MG	DA	9570	1/1	0.31	-	61,61,61,61	0
57	MG	CA	1712	1/1	0.23	-	34,34,34,34	1
57	MG	DA	9602	1/1	0.55	-	37,37,37,37	0
57	MG	BA	3068	1/1	0.12	-	11,11,11,11	0
57	MG	CA	1702	1/1	0.12	-	49,49,49,49	0
57	MG	DA	9447	1/1	0.23	-	68,68,68,68	0
57	MG	DA	9696	1/1	0.45	-	34,34,34,34	0
57	MG	BA	3127	1/1	0.40	-	8,8,8,8	0
57	MG	BA	3164	1/1	0.41	-	39,39,39,39	0
57	MG	DA	9653	1/1	0.44	-	5,5,5,5	0
57	MG	DA	9679	1/1	0.33	-	16,16,16,16	0
57	MG	AA	7071	1/1	0.55	-	38,38,38,38	0
57	MG	AA	7066	1/1	0.51	-	36,36,36,36	0
57	MG	BA	3252	1/1	0.48	-	56,56,56,56	0
57	MG	AV	104	1/1	0.42	-	16,16,16,16	0
57	MG	BA	3319	1/1	0.30	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9431	1/1	0.31	-	12,12,12,12	0
57	MG	DA	9610	1/1	0.68	-	19,19,19,19	0
57	MG	DA	9316	1/1	0.24	-	0,0,0,0	0
57	MG	CA	1655	1/1	0.49	-	24,24,24,24	0
57	MG	BA	3098	1/1	0.29	-	36,36,36,36	0
57	MG	BA	3154	1/1	0.46	-	17,17,17,17	0
57	MG	DA	9361	1/1	0.34	-	5,5,5,5	0
57	MG	DA	9436	1/1	0.52	-	3,3,3,3	0
57	MG	BA	3125	1/1	0.31	-	20,20,20,20	0
57	MG	CA	1622	1/1	0.09	-	37,37,37,37	0
57	MG	BA	3269	1/1	0.50	-	20,20,20,20	0
57	MG	CA	1733	1/1	0.44	-	11,11,11,11	0
57	MG	CA	1671	1/1	0.21	-	38,38,38,38	0
57	MG	DA	9630	1/1	0.25	-	16,16,16,16	1
57	MG	CA	1625	1/1	0.42	-	26,26,26,26	0
57	MG	D1	101	1/1	0.75	-	55,55,55,55	0
57	MG	BA	3145	1/1	0.30	-	22,22,22,22	0
57	MG	DA	9690	1/1	0.12	-	5,5,5,5	0
57	MG	BA	3091	1/1	0.22	-	0,0,0,0	0
57	MG	BA	3117	1/1	0.70	-	11,11,11,11	1
57	MG	BA	3159	1/1	0.50	-	9,9,9,9	0
57	MG	DA	9554	1/1	0.28	-	10,10,10,10	0
57	MG	BA	3292	1/1	0.30	-	28,28,28,28	0
57	MG	CA	1652	1/1	0.61	-	6,6,6,6	0
57	MG	DA	9474	1/1	0.28	-	28,28,28,28	0
57	MG	DA	9432	1/1	0.63	-	38,38,38,38	0
57	MG	DA	9349	1/1	0.63	-	3,3,3,3	0
57	MG	AA	7040	1/1	0.16	-	36,36,36,36	0
57	MG	BA	3307	1/1	0.56	-	25,25,25,25	0
57	MG	CA	1681	1/1	0.75	-	18,18,18,18	1
57	MG	BA	3111	1/1	0.33	-	35,35,35,35	0
57	MG	CA	1726	1/1	0.21	-	38,38,38,38	0
57	MG	DA	9669	1/1	0.19	-	5,5,5,5	0
57	MG	BA	3026	1/1	0.52	-	29,29,29,29	0
57	MG	DA	9476	1/1	0.45	-	2,2,2,2	0
57	MG	AA	7093	1/1	0.36	-	30,30,30,30	0
57	MG	AA	7042	1/1	0.08	-	31,31,31,31	0
57	MG	CA	1630	1/1	0.25	-	34,34,34,34	0
57	MG	CA	1663	1/1	0.65	-	11,11,11,11	0
57	MG	DA	9516	1/1	0.47	-	1,1,1,1	0
57	MG	DA	9627	1/1	0.33	-	0,0,0,0	1
57	MG	CA	1636	1/1	0.34	-	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
57	MG	BA	3042	1/1	0.68	-	8,8,8,8	0
57	MG	DA	9497	1/1	0.35	-	29,29,29,29	0
57	MG	DA	9510	1/1	0.55	-	1,1,1,1	0
57	MG	DA	9661	1/1	0.39	-	57,57,57,57	0
57	MG	DA	9421	1/1	0.39	-	28,28,28,28	0
57	MG	CA	1734	1/1	0.20	-	22,22,22,22	0
57	MG	DA	9670	1/1	0.47	-	11,11,11,11	0
57	MG	DA	9364	1/1	0.82	-	1,1,1,1	0
57	MG	BA	3263	1/1	0.60	-	16,16,16,16	1
57	MG	AA	7058	1/1	0.28	-	13,13,13,13	0
57	MG	DA	9377	1/1	0.19	-	19,19,19,19	0
57	MG	D0	101	1/1	0.46	-	27,27,27,27	0
57	MG	BA	3025	1/1	0.15	-	37,37,37,37	0
57	MG	BA	3009	1/1	0.14	-	2,2,2,2	0
57	MG	CE	202	1/1	0.32	-	34,34,34,34	0
57	MG	DA	9556	1/1	0.23	-	23,23,23,23	0
57	MG	AA	7001	1/1	0.28	-	26,26,26,26	0
57	MG	BA	3046	1/1	0.60	-	1,1,1,1	0
57	MG	CA	1646	1/1	0.41	-	7,7,7,7	0
57	MG	DA	9640	1/1	0.38	-	42,42,42,42	0
57	MG	DA	9506	1/1	0.25	-	0,0,0,0	0
57	MG	BA	3060	1/1	0.58	-	1,1,1,1	0
57	MG	DA	9337	1/1	0.59	-	45,45,45,45	0
57	MG	BA	3077	1/1	0.43	-	21,21,21,21	0
57	MG	DA	9629	1/1	0.18	-	52,52,52,52	0
57	MG	DA	9444	1/1	0.48	-	42,42,42,42	0
57	MG	DA	9414	1/1	0.81	-	16,16,16,16	0
57	MG	DA	9453	1/1	0.47	-	4,4,4,4	1
57	MG	DU	202	1/1	0.15	-	6,6,6,6	0
57	MG	BA	3020	1/1	0.46	-	1,1,1,1	0
57	MG	BA	3203	1/1	0.47	-	37,37,37,37	0
57	MG	DA	9563	1/1	0.26	-	3,3,3,3	0
57	MG	BA	3133	1/1	0.23	-	43,43,43,43	0
57	MG	BA	3287	1/1	0.40	-	30,30,30,30	0
57	MG	AA	7068	1/1	0.09	-	34,34,34,34	0
57	MG	CA	1653	1/1	0.58	-	29,29,29,29	0
57	MG	BA	3312	1/1	0.35	-	45,45,45,45	0
57	MG	DA	9434	1/1	0.42	-	4,4,4,4	0
57	MG	DA	9484	1/1	0.39	-	5,5,5,5	0
57	MG	BA	3034	1/1	0.20	-	7,7,7,7	0
57	MG	DA	9383	1/1	0.37	-	18,18,18,18	0
57	MG	BA	3173	1/1	0.60	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DD	7102	1/1	0.27	-	0,0,0,0	0
57	MG	BA	3142	1/1	0.43	-	10,10,10,10	0
57	MG	CA	1674	1/1	0.47	-	89,89,89,89	0
57	MG	DA	9486	1/1	0.36	-	21,21,21,21	0
57	MG	DA	9536	1/1	0.44	-	0,0,0,0	0
57	MG	BA	3085	1/1	0.25	-	29,29,29,29	0
57	MG	AA	7030	1/1	0.22	-	2,2,2,2	0
57	MG	DA	9329	1/1	0.47	-	21,21,21,21	0
57	MG	DA	9551	1/1	0.20	-	48,48,48,48	0
57	MG	BA	3245	1/1	0.69	-	45,45,45,45	0
57	MG	CA	1619	1/1	0.56	-	11,11,11,11	0
57	MG	BB	205	1/1	0.12	-	19,19,19,19	1
57	MG	DA	9473	1/1	0.68	-	0,0,0,0	0
57	MG	AA	7096	1/1	0.55	-	31,31,31,31	0
57	MG	BA	3087	1/1	0.23	-	21,21,21,21	0
57	MG	CA	1713	1/1	0.53	-	31,31,31,31	0
57	MG	AA	7056	1/1	0.34	-	12,12,12,12	0
57	MG	DA	9652	1/1	0.22	-	44,44,44,44	0
57	MG	AA	7067	1/1	0.47	-	28,28,28,28	0
57	MG	BA	3090	1/1	0.40	-	2,2,2,2	0
57	MG	DA	9687	1/1	0.29	-	12,12,12,12	0
57	MG	DA	9313	1/1	0.22	-	18,18,18,18	0
57	MG	CA	1611	1/1	0.54	-	0,0,0,0	0
57	MG	CA	1629	1/1	0.34	-	37,37,37,37	0
57	MG	DA	9416	1/1	0.32	-	38,38,38,38	0
57	MG	BA	3048	1/1	0.31	-	17,17,17,17	0
57	MG	DA	9583	1/1	0.18	-	1,1,1,1	0
57	MG	DA	9631	1/1	0.32	-	21,21,21,21	0
57	MG	CA	1693	1/1	0.41	-	24,24,24,24	0
57	MG	DA	9427	1/1	0.21	-	91,91,91,91	0
57	MG	CA	1654	1/1	0.39	-	31,31,31,31	0
57	MG	BA	3187	1/1	0.61	-	24,24,24,24	0
57	MG	AA	7006	1/1	0.39	-	20,20,20,20	0
57	MG	DA	9390	1/1	0.28	-	0,0,0,0	0
57	MG	DA	9346	1/1	0.28	-	0,0,0,0	0
57	MG	BA	3215	1/1	0.39	-	1,1,1,1	0
57	MG	DA	9456	1/1	0.62	-	19,19,19,19	0
57	MG	DA	9304	1/1	0.39	-	27,27,27,27	0
57	MG	CA	1689	1/1	0.22	-	15,15,15,15	0
57	MG	DA	9441	1/1	0.65	-	31,31,31,31	1
57	MG	AV	101	1/1	0.14	-	2,2,2,2	0
57	MG	DA	9401	1/1	0.54	-	21,21,21,21	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9512	1/1	0.41	-	2,2,2,2	0
57	MG	DA	9397	1/1	0.40	-	25,25,25,25	1
57	MG	BA	3320	1/1	0.44	-	54,54,54,54	0
57	MG	CV	103	1/1	0.30	-	43,43,43,43	1
57	MG	BA	3256	1/1	0.16	-	13,13,13,13	0
57	MG	DA	9402	1/1	0.38	-	25,25,25,25	0
57	MG	CA	1624	1/1	0.32	-	18,18,18,18	0
57	MG	BA	3301	1/1	0.27	-	20,20,20,20	0
57	MG	CA	1703	1/1	0.45	-	9,9,9,9	0
57	MG	BA	3116	1/1	0.29	-	38,38,38,38	0
57	MG	AA	7064	1/1	0.32	-	50,50,50,50	0
57	MG	BA	3059	1/1	0.16	-	0,0,0,0	0
57	MG	DP	203	1/1	0.22	-	11,11,11,11	0
57	MG	BA	3186	1/1	0.34	-	2,2,2,2	0
57	MG	DA	9392	1/1	0.67	-	12,12,12,12	0
57	MG	DA	9643	1/1	0.65	-	34,34,34,34	1
57	MG	AA	7034	1/1	0.78	-	43,43,43,43	0
57	MG	BA	3267	1/1	0.42	-	41,41,41,41	0
57	MG	BA	3019	1/1	0.32	-	44,44,44,44	0
57	MG	DA	9543	1/1	0.32	-	5,5,5,5	0
57	MG	AA	7086	1/1	0.97	-	30,30,30,30	0
57	MG	DA	9495	1/1	0.74	-	3,3,3,3	0
57	MG	BA	3260	1/1	0.59	-	8,8,8,8	0
57	MG	BA	3172	1/1	0.26	-	58,58,58,58	0
57	MG	DA	9553	1/1	0.36	-	20,20,20,20	0
57	MG	BA	3066	1/1	0.25	-	48,48,48,48	0
57	MG	DA	9597	1/1	0.24	-	12,12,12,12	0
57	MG	AA	7032	1/1	0.47	-	24,24,24,24	0
57	MG	BA	3089	1/1	0.23	-	18,18,18,18	0
57	MG	CA	1742	1/1	0.46	-	10,10,10,10	0
57	MG	DA	9594	1/1	0.74	-	19,19,19,19	0
57	MG	DA	9635	1/1	0.56	-	24,24,24,24	0
57	MG	BA	3012	1/1	0.62	-	29,29,29,29	0
57	MG	BA	3112	1/1	0.58	-	14,14,14,14	0
57	MG	DA	9321	1/1	0.51	-	35,35,35,35	0
57	MG	D1	102	1/1	0.17	-	9,9,9,9	1
57	MG	DA	9359	1/1	0.37	-	0,0,0,0	0
57	MG	AA	7053	1/1	0.50	-	32,32,32,32	0
57	MG	DA	9499	1/1	0.16	-	29,29,29,29	0
57	MG	BA	3227	1/1	0.69	-	40,40,40,40	0
57	MG	DA	9435	1/1	0.95	-	30,30,30,30	0
57	MG	BA	3002	1/1	0.26	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	7043	1/1	0.36	-	16,16,16,16	0
57	MG	CA	1637	1/1	0.35	-	57,57,57,57	0
57	MG	BA	3144	1/1	0.71	-	41,41,41,41	0
57	MG	AA	7051	1/1	0.41	-	22,22,22,22	0
57	MG	CA	1627	1/1	0.61	-	22,22,22,22	0
57	MG	DA	9573	1/1	0.40	-	45,45,45,45	0
57	MG	BA	3271	1/1	0.70	-	52,52,52,52	0
57	MG	CA	1687	1/1	0.32	-	47,47,47,47	0
57	MG	AA	7033	1/1	0.21	-	35,35,35,35	0
57	MG	AA	7090	1/1	1.13	-	69,69,69,69	0
57	MG	AA	7089	1/1	0.27	-	21,21,21,21	0
57	MG	BA	3189	1/1	0.46	-	1,1,1,1	0
57	MG	B5	101	1/1	0.30	-	2,2,2,2	0
57	MG	BA	3084	1/1	0.48	-	1,1,1,1	0
57	MG	DA	9617	1/1	0.31	-	11,11,11,11	0
57	MG	BA	3138	1/1	0.33	-	15,15,15,15	0
57	MG	BA	3277	1/1	0.62	-	2,2,2,2	1
57	MG	BA	3197	1/1	0.22	-	1,1,1,1	0
57	MG	AA	7102	1/1	0.50	-	38,38,38,38	0
57	MG	DA	9319	1/1	0.79	-	30,30,30,30	0
57	MG	CA	1672	1/1	0.53	-	62,62,62,62	0
57	MG	DA	9437	1/1	0.20	-	14,14,14,14	0
57	MG	BA	3104	1/1	0.22	-	16,16,16,16	0
57	MG	BA	3101	1/1	1.30	-	27,27,27,27	1
57	MG	CA	1706	1/1	0.35	-	32,32,32,32	0
57	MG	DA	9446	1/1	0.09	-	13,13,13,13	0
57	MG	DA	9439	1/1	0.24	-	32,32,32,32	0
57	MG	DA	9306	1/1	0.35	-	4,4,4,4	0
57	MG	DA	9693	1/1	0.99	-	47,47,47,47	0
57	MG	CA	1616	1/1	0.39	-	44,44,44,44	0
57	MG	DA	9681	1/1	0.36	-	13,13,13,13	0
57	MG	BA	3218	1/1	0.32	-	24,24,24,24	0
57	MG	CA	1690	1/1	0.57	-	17,17,17,17	0
57	MG	BA	3258	1/1	1.04	-	19,19,19,19	0
57	MG	CA	1683	1/1	0.29	-	29,29,29,29	0
57	MG	DA	9672	1/1	0.36	-	5,5,5,5	0
57	MG	BA	3289	1/1	0.55	-	21,21,21,21	0
57	MG	CA	1721	1/1	0.20	-	1,1,1,1	0
57	MG	BA	3008	1/1	0.46	-	2,2,2,2	0
57	MG	DA	9692	1/1	0.46	-	30,30,30,30	0
57	MG	BA	3071	1/1	0.33	-	0,0,0,0	0
57	MG	DE	301	1/1	0.31	-	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9579	1/1	0.71	-	38,38,38,38	0
57	MG	CA	1684	1/1	0.21	-	41,41,41,41	0
57	MG	DA	9343	1/1	0.26	-	2,2,2,2	0
57	MG	BA	3201	1/1	0.32	-	6,6,6,6	0
57	MG	DA	9420	1/1	0.53	-	6,6,6,6	0
57	MG	DA	9386	1/1	0.42	-	2,2,2,2	0
57	MG	DA	9480	1/1	0.26	-	30,30,30,30	0
57	MG	DA	9433	1/1	0.20	-	13,13,13,13	0
57	MG	BA	3206	1/1	0.44	-	29,29,29,29	0
57	MG	DA	9586	1/1	0.24	-	3,3,3,3	0
57	MG	DP	202	1/1	0.26	-	173,173,173,173	0
57	MG	DB	201	1/1	0.41	-	22,22,22,22	0
57	MG	DA	9462	1/1	0.48	-	30,30,30,30	0
57	MG	BA	3036	1/1	0.20	-	78,78,78,78	1
57	MG	DA	9532	1/1	0.45	-	9,9,9,9	0
57	MG	DA	9301	1/1	0.33	-	32,32,32,32	0
57	MG	DA	9411	1/1	0.26	-	2,2,2,2	0
57	MG	AA	7002	1/1	0.48	-	35,35,35,35	0
57	MG	AA	7016	1/1	0.30	-	45,45,45,45	0
57	MG	DA	9325	1/1	0.50	-	32,32,32,32	0
57	MG	BA	3051	1/1	0.43	-	6,6,6,6	0
57	MG	BA	3298	1/1	0.76	-	18,18,18,18	0
57	MG	BA	3251	1/1	0.23	-	34,34,34,34	0
57	MG	AA	7079	1/1	0.40	-	35,35,35,35	0
57	MG	DA	9538	1/1	0.45	-	1,1,1,1	0
57	MG	DA	9312	1/1	0.66	-	4,4,4,4	0
57	MG	BA	3221	1/1	0.73	-	17,17,17,17	0
57	MG	BA	3208	1/1	0.21	-	8,8,8,8	0
57	MG	DD	7103	1/1	0.39	-	0,0,0,0	0
57	MG	CW	101	1/1	0.52	-	29,29,29,29	1
57	MG	DA	9513	1/1	0.48	-	22,22,22,22	0
57	MG	CA	1618	1/1	0.15	-	31,31,31,31	0
57	MG	DA	9633	1/1	0.75	-	30,30,30,30	0
57	MG	DA	9666	1/1	0.37	-	7,7,7,7	0
57	MG	D5	102	1/1	0.28	-	32,32,32,32	1
57	MG	BA	3156	1/1	0.33	-	19,19,19,19	0
57	MG	DA	9609	1/1	0.46	-	2,2,2,2	0
57	MG	DA	9540	1/1	0.35	-	0,0,0,0	0
57	MG	BA	3212	1/1	0.26	-	8,8,8,8	0
57	MG	BA	3250	1/1	0.29	-	18,18,18,18	0
57	MG	CA	1714	1/1	0.45	-	53,53,53,53	0
57	MG	DA	9621	1/1	0.56	-	0,0,0,0	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3281	1/1	0.65	-	53,53,53,53	0
57	MG	BA	3239	1/1	0.36	-	1,1,1,1	0
57	MG	BE	302	1/1	0.30	-	74,74,74,74	0
57	MG	BA	3228	1/1	0.61	-	13,13,13,13	0
57	MG	CA	1695	1/1	0.38	-	15,15,15,15	0
57	MG	DA	9664	1/1	0.52	-	1,1,1,1	0
57	MG	BA	3191	1/1	0.44	-	2,2,2,2	0
57	MG	DP	201	1/1	0.12	-	7,7,7,7	0
57	MG	AA	7100	1/1	0.81	-	21,21,21,21	0
57	MG	DA	9603	1/1	0.87	-	33,33,33,33	0
57	MG	BA	3196	1/1	0.78	-	30,30,30,30	0
57	MG	DA	9393	1/1	0.30	-	24,24,24,24	0
57	MG	AA	7018	1/1	0.58	-	27,27,27,27	0
57	MG	BA	3153	1/1	0.52	-	0,0,0,0	0
57	MG	CA	1638	1/1	0.46	-	24,24,24,24	0
57	MG	CA	1620	1/1	0.25	-	1,1,1,1	0
57	MG	BA	3013	1/1	0.32	-	16,16,16,16	0
57	MG	CA	1676	1/1	0.62	-	88,88,88,88	0
57	MG	DA	9403	1/1	0.25	-	0,0,0,0	0
57	MG	DA	9650	1/1	0.24	-	7,7,7,7	0
57	MG	DA	9372	1/1	0.46	-	8,8,8,8	0
57	MG	DA	9309	1/1	0.34	-	6,6,6,6	0
57	MG	DA	9352	1/1	0.23	-	89,89,89,89	0
57	MG	DA	9612	1/1	0.64	-	1,1,1,1	1
57	MG	CA	1719	1/1	0.36	-	10,10,10,10	0
57	MG	DA	9466	1/1	0.43	-	36,36,36,36	0
57	MG	BA	3058	1/1	0.33	-	1,1,1,1	0
57	MG	BA	3311	1/1	0.41	-	13,13,13,13	0
57	MG	DA	9634	1/1	0.39	-	44,44,44,44	0
57	MG	DA	9624	1/1	0.28	-	18,18,18,18	1
57	MG	AA	7099	1/1	0.37	-	6,6,6,6	0
57	MG	DA	9460	1/1	0.25	-	40,40,40,40	0
57	MG	CA	1661	1/1	0.35	-	50,50,50,50	0
57	MG	CV	101	1/1	0.38	-	12,12,12,12	1
57	MG	DA	9595	1/1	0.67	-	49,49,49,49	0
57	MG	CA	1728	1/1	0.34	-	59,59,59,59	0
57	MG	CA	1651	1/1	0.46	-	39,39,39,39	0
57	MG	DA	9658	1/1	0.20	-	36,36,36,36	0
57	MG	CA	1617	1/1	0.42	-	16,16,16,16	0
57	MG	BA	3240	1/1	0.15	-	21,21,21,21	0
57	MG	AA	7062	1/1	0.11	-	31,31,31,31	0
57	MG	BA	3322	1/1	0.38	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9360	1/1	0.37	-	7,7,7,7	0
57	MG	BA	3286	1/1	0.25	-	22,22,22,22	0
57	MG	BA	3010	1/1	0.88	-	28,28,28,28	0
57	MG	AA	7076	1/1	0.57	-	60,60,60,60	0
57	MG	AA	7005	1/1	0.26	-	45,45,45,45	0
57	MG	DA	9572	1/1	0.43	-	4,4,4,4	0
57	MG	BA	3140	1/1	0.23	-	40,40,40,40	0
57	MG	DA	9426	1/1	0.46	-	9,9,9,9	1
57	MG	BA	3128	1/1	0.26	-	57,57,57,57	0
57	MG	DA	9362	1/1	0.35	-	5,5,5,5	0
57	MG	BA	3262	1/1	0.61	-	39,39,39,39	0
57	MG	BA	3064	1/1	0.24	-	29,29,29,29	1
57	MG	BA	3030	1/1	0.54	-	22,22,22,22	0
57	MG	DA	9565	1/1	0.37	-	11,11,11,11	0
57	MG	DA	9505	1/1	0.29	-	0,0,0,0	0
57	MG	DA	9417	1/1	0.30	-	20,20,20,20	0
57	MG	BA	3110	1/1	0.60	-	23,23,23,23	1
57	MG	BA	3108	1/1	0.28	-	27,27,27,27	0
57	MG	AA	7027	1/1	0.43	-	28,28,28,28	0
57	MG	BA	3270	1/1	0.48	-	0,0,0,0	1
57	MG	BA	3306	1/1	0.46	-	48,48,48,48	0
57	MG	BA	3282	1/1	0.44	-	24,24,24,24	0
57	MG	DA	9340	1/1	0.33	-	1,1,1,1	0
57	MG	AA	7044	1/1	0.36	-	21,21,21,21	0
57	MG	BA	3062	1/1	0.15	-	27,27,27,27	0
57	MG	DA	9458	1/1	0.42	-	22,22,22,22	0
57	MG	BA	3092	1/1	0.19	-	1,1,1,1	0
57	MG	DA	9303	1/1	0.29	-	42,42,42,42	0
57	MG	AA	7021	1/1	0.31	-	25,25,25,25	0
57	MG	BA	3193	1/1	0.46	-	12,12,12,12	0
57	MG	AA	7085	1/1	0.17	-	15,15,15,15	0
57	MG	BA	3234	1/1	0.56	-	10,10,10,10	0
57	MG	AA	7007	1/1	0.13	-	1,1,1,1	0
57	MG	BA	3027	1/1	0.36	-	4,4,4,4	0
57	MG	DA	9593	1/1	0.62	-	25,25,25,25	0
57	MG	BA	3069	1/1	0.34	-	5,5,5,5	0
57	MG	AA	7014	1/1	0.92	-	20,20,20,20	0
57	MG	BA	3050	1/1	0.56	-	4,4,4,4	0
57	MG	BA	3253	1/1	0.60	-	34,34,34,34	0
57	MG	BA	3039	1/1	0.44	-	30,30,30,30	0
57	MG	CA	1705	1/1	0.21	-	15,15,15,15	0
57	MG	D2	101	1/1	0.23	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DB	203	1/1	0.95	-	1,1,1,1	1
57	MG	AA	7035	1/1	0.13	-	42,42,42,42	0
57	MG	DA	9574	1/1	0.42	-	14,14,14,14	1
57	MG	CA	1707	1/1	0.82	-	1,1,1,1	1
57	MG	BA	3102	1/1	0.50	-	1,1,1,1	0
57	MG	DA	9428	1/1	0.40	-	15,15,15,15	0
57	MG	CA	1738	1/1	0.39	-	49,49,49,49	0
57	MG	BA	3088	1/1	0.39	-	43,43,43,43	0
57	MG	BA	3131	1/1	0.40	-	38,38,38,38	0
57	MG	DA	9339	1/1	0.23	-	13,13,13,13	0
57	MG	DA	9659	1/1	0.27	-	52,52,52,52	0
57	MG	BA	3126	1/1	0.60	-	44,44,44,44	0
57	MG	DA	9358	1/1	0.45	-	5,5,5,5	0
57	MG	BA	3083	1/1	0.31	-	27,27,27,27	1
57	MG	CA	1670	1/1	0.40	-	2,2,2,2	0
57	MG	CA	1730	1/1	0.16	-	49,49,49,49	0
57	MG	DA	9619	1/1	0.14	-	0,0,0,0	0
57	MG	CA	1606	1/1	0.21	-	8,8,8,8	0
57	MG	CA	1643	1/1	0.53	-	40,40,40,40	1
57	MG	BA	3158	1/1	0.38	-	29,29,29,29	0
57	MG	DA	9310	1/1	0.29	-	0,0,0,0	0
57	MG	DA	9644	1/1	0.15	-	25,25,25,25	0
57	MG	DA	9547	1/1	0.24	-	3,3,3,3	0
57	MG	DA	9684	1/1	0.25	-	8,8,8,8	0
57	MG	CA	1677	1/1	0.19	-	22,22,22,22	0
57	MG	CA	1639	1/1	0.71	-	55,55,55,55	0
57	MG	DA	9398	1/1	0.42	-	0,0,0,0	0
57	MG	DA	9623	1/1	0.37	-	13,13,13,13	0
57	MG	DA	9452	1/1	0.36	-	10,10,10,10	0
57	MG	DA	9555	1/1	0.30	-	39,39,39,39	0
57	MG	DA	9683	1/1	0.51	-	19,19,19,19	0
57	MG	DA	9514	1/1	0.87	-	19,19,19,19	0
57	MG	BA	3005	1/1	0.26	-	22,22,22,22	0
57	MG	BA	3097	1/1	0.25	-	43,43,43,43	0
57	MG	DA	9592	1/1	0.16	-	36,36,36,36	0
57	MG	BA	3316	1/1	0.41	-	7,7,7,7	0
57	MG	CA	1710	1/1	0.53	-	19,19,19,19	0
57	MG	CE	201	1/1	0.65	-	16,16,16,16	0
57	MG	DA	9369	1/1	0.60	-	0,0,0,0	0
57	MG	AX	101	1/1	0.26	-	43,43,43,43	0
57	MG	BA	3016	1/1	0.34	-	8,8,8,8	0
57	MG	CA	1694	1/1	0.76	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3244	1/1	0.14	-	1,1,1,1	0
57	MG	AA	7041	1/1	0.55	-	20,20,20,20	0
57	MG	BA	3217	1/1	0.18	-	28,28,28,28	0
57	MG	BA	3166	1/1	0.63	-	40,40,40,40	0
57	MG	BA	3053	1/1	0.29	-	17,17,17,17	0
57	MG	BA	3081	1/1	0.87	-	24,24,24,24	1
57	MG	DA	9697	1/1	0.22	-	41,41,41,41	0
57	MG	BA	3219	1/1	0.22	-	19,19,19,19	0
57	MG	DA	9320	1/1	0.25	-	10,10,10,10	0
57	MG	DA	9324	1/1	0.48	-	2,2,2,2	0
57	MG	BA	3072	1/1	0.19	-	25,25,25,25	0
57	MG	BA	3149	1/1	0.32	-	27,27,27,27	0
57	MG	BA	3094	1/1	0.35	-	7,7,7,7	0
57	MG	DA	9370	1/1	0.41	-	0,0,0,0	0
57	MG	AA	7023	1/1	0.27	-	56,56,56,56	0
57	MG	DA	9481	1/1	0.08	-	0,0,0,0	0
57	MG	DA	9641	1/1	0.10	-	11,11,11,11	0
57	MG	DA	9678	1/1	0.23	-	33,33,33,33	0
57	MG	BA	3157	1/1	0.23	-	6,6,6,6	0
57	MG	CA	1697	1/1	0.17	-	49,49,49,49	0
57	MG	BA	3323	1/1	0.46	-	26,26,26,26	0
57	MG	DA	9560	1/1	0.28	-	4,4,4,4	0
57	MG	BB	202	1/1	0.15	-	62,62,62,62	0
57	MG	CA	1708	1/1	0.67	-	34,34,34,34	0
57	MG	AA	7069	1/1	0.62	-	11,11,11,11	1
57	MG	AA	7052	1/1	0.22	-	74,74,74,74	0
57	MG	BD	301	1/1	0.56	-	7,7,7,7	0
57	MG	CA	1701	1/1	0.53	-	1,1,1,1	0
57	MG	DA	9676	1/1	0.23	-	13,13,13,13	0
57	MG	DA	9585	1/1	0.17	-	18,18,18,18	0
57	MG	DA	9379	1/1	0.31	-	41,41,41,41	0
57	MG	DA	9405	1/1	0.30	-	5,5,5,5	0
57	MG	BA	3318	1/1	0.46	-	37,37,37,37	0
57	MG	BD	302	1/1	0.23	-	4,4,4,4	0
57	MG	DA	9668	1/1	0.52	-	4,4,4,4	0
57	MG	DA	9537	1/1	0.34	-	0,0,0,0	0
57	MG	DA	9566	1/1	0.32	-	18,18,18,18	0
57	MG	AA	7092	1/1	0.12	-	37,37,37,37	0
57	MG	DA	9491	1/1	0.42	-	11,11,11,11	0
57	MG	BA	3194	1/1	0.30	-	1,1,1,1	0
57	MG	DA	9674	1/1	0.81	-	17,17,17,17	0
57	MG	BA	3237	1/1	0.23	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1720	1/1	0.41	-	2,2,2,2	0
57	MG	CA	1685	1/1	0.42	-	41,41,41,41	0
57	MG	DA	9559	1/1	0.53	-	58,58,58,58	0
57	MG	DA	9686	1/1	0.21	-	11,11,11,11	0
57	MG	BA	3283	1/1	0.20	-	22,22,22,22	0
57	MG	BA	3063	1/1	0.53	-	55,55,55,55	0
57	MG	DA	9523	1/1	0.76	-	9,9,9,9	0
57	MG	BA	3280	1/1	0.24	-	19,19,19,19	1
57	MG	DA	9625	1/1	0.38	-	26,26,26,26	0
57	MG	CA	1660	1/1	0.35	-	9,9,9,9	0
57	MG	DA	9347	1/1	0.29	-	22,22,22,22	0
57	MG	DQ	201	1/1	0.34	-	36,36,36,36	0
57	MG	BA	3309	1/1	0.78	-	25,25,25,25	0
57	MG	AA	7070	1/1	0.18	-	61,61,61,61	0
57	MG	DA	9376	1/1	0.27	-	26,26,26,26	0
57	MG	DA	9323	1/1	0.54	-	33,33,33,33	0
57	MG	BA	3231	1/1	0.38	-	90,90,90,90	0
57	MG	CA	1736	1/1	0.32	-	6,6,6,6	0
57	MG	BA	3188	1/1	0.33	-	0,0,0,0	0
57	MG	BA	3297	1/1	0.95	-	46,46,46,46	0
57	MG	DA	9371	1/1	0.38	-	29,29,29,29	0
57	MG	DA	9415	1/1	0.49	-	0,0,0,0	0
57	MG	BA	3045	1/1	0.58	-	2,2,2,2	0
57	MG	DA	9509	1/1	0.44	-	17,17,17,17	0
57	MG	BA	3029	1/1	0.12	-	24,24,24,24	0
57	MG	AV	102	1/1	0.44	-	25,25,25,25	1
57	MG	BA	3095	1/1	1.00	-	35,35,35,35	0
57	MG	DA	9396	1/1	0.26	-	26,26,26,26	0
57	MG	DA	9535	1/1	0.42	-	14,14,14,14	0
57	MG	DA	9689	1/1	0.83	-	25,25,25,25	0
57	MG	CA	1626	1/1	0.54	-	28,28,28,28	0
57	MG	AA	7094	1/1	0.54	-	8,8,8,8	0
57	MG	DA	9600	1/1	0.34	-	55,55,55,55	0
57	MG	BA	3295	1/1	0.35	-	27,27,27,27	0
57	MG	DA	9608	1/1	0.49	-	19,19,19,19	0
57	MG	DA	9467	1/1	0.44	-	53,53,53,53	1
57	MG	BA	3238	1/1	0.35	-	9,9,9,9	0
57	MG	CA	1729	1/1	0.39	-	35,35,35,35	0
57	MG	DA	9545	1/1	0.43	-	1,1,1,1	0
57	MG	BA	3021	1/1	0.56	-	49,49,49,49	0
57	MG	BA	3003	1/1	0.30	-	33,33,33,33	0
57	MG	BA	3161	1/1	0.26	-	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9496	1/1	0.40	-	26,26,26,26	0
57	MG	BA	3035	1/1	0.37	-	0,0,0,0	0
57	MG	BA	3143	1/1	0.22	-	7,7,7,7	0
57	MG	CA	1650	1/1	0.51	-	34,34,34,34	0
57	MG	DA	9429	1/1	0.89	-	51,51,51,51	0
57	MG	DA	9489	1/1	0.41	-	37,37,37,37	0
57	MG	AA	7087	1/1	0.12	-	24,24,24,24	0
57	MG	AA	7074	1/1	0.77	-	26,26,26,26	0
57	MG	BA	3103	1/1	0.24	-	31,31,31,31	0
57	MG	DA	9400	1/1	0.41	-	0,0,0,0	0
57	MG	CA	1608	1/1	0.38	-	16,16,16,16	0
57	MG	BA	3204	1/1	0.32	-	3,3,3,3	0
57	MG	DA	9318	1/1	0.39	-	2,2,2,2	0
57	MG	DA	9353	1/1	0.57	-	24,24,24,24	0
57	MG	BA	3200	1/1	0.54	-	5,5,5,5	0
57	MG	DA	9526	1/1	0.51	-	12,12,12,12	0
57	MG	AA	7073	1/1	0.21	-	29,29,29,29	0
57	MG	DA	9388	1/1	0.19	-	28,28,28,28	0
57	MG	BA	3246	1/1	0.64	-	33,33,33,33	0
57	MG	BA	3278	1/1	0.40	-	22,22,22,22	0
57	MG	BA	3226	1/1	0.67	-	36,36,36,36	0
57	MG	CA	1635	1/1	0.25	-	4,4,4,4	0
57	MG	CA	1682	1/1	0.28	-	60,60,60,60	0
57	MG	DA	9519	1/1	0.43	-	1,1,1,1	0
57	MG	AA	7098	1/1	0.34	-	28,28,28,28	0
57	MG	DA	9517	1/1	0.31	-	0,0,0,0	0
57	MG	DA	9651	1/1	0.14	-	81,81,81,81	0
57	MG	CA	1628	1/1	0.23	-	9,9,9,9	0
57	MG	BA	3209	1/1	0.36	-	1,1,1,1	0
57	MG	BA	3086	1/1	0.25	-	1,1,1,1	0
57	MG	BU	201	1/1	0.32	-	170,170,170,170	1
57	MG	CA	1680	1/1	0.15	-	49,49,49,49	0
57	MG	CA	1641	1/1	0.21	-	40,40,40,40	0
57	MG	CA	1665	1/1	0.41	-	16,16,16,16	0
57	MG	DA	9515	1/1	0.34	-	10,10,10,10	0
57	MG	DA	9471	1/1	0.55	-	50,50,50,50	1
57	MG	AA	7110	1/1	0.36	-	31,31,31,31	0
57	MG	DA	9341	1/1	0.55	-	11,11,11,11	0
57	MG	DA	9685	1/1	0.59	-	22,22,22,22	0
57	MG	CA	1658	1/1	0.34	-	44,44,44,44	0
57	MG	AA	7011	1/1	0.40	-	43,43,43,43	0
57	MG	DA	9381	1/1	0.24	-	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9399	1/1	0.73	-	52,52,52,52	0
57	MG	BA	3129	1/1	0.53	-	1,1,1,1	0
57	MG	BA	3041	1/1	0.49	-	7,7,7,7	0
57	MG	BA	3314	1/1	0.05	-	42,42,42,42	0
57	MG	AA	7091	1/1	0.29	-	22,22,22,22	0
57	MG	BA	3213	1/1	0.44	-	8,8,8,8	0
57	MG	AA	7022	1/1	0.24	-	32,32,32,32	0
57	MG	BA	3004	1/1	0.58	-	1,1,1,1	0
57	MG	DA	9576	1/1	0.42	-	22,22,22,22	0
57	MG	CA	1725	1/1	0.31	-	29,29,29,29	0
57	MG	CA	1698	1/1	0.14	-	1,1,1,1	1
57	MG	CA	1715	1/1	0.48	-	12,12,12,12	0
57	MG	BA	3255	1/1	0.44	-	45,45,45,45	0
57	MG	BA	3296	1/1	0.41	-	0,0,0,0	1
57	MG	DA	9656	1/1	0.23	-	58,58,58,58	0
57	MG	DA	9308	1/1	0.45	-	2,2,2,2	0
57	MG	CA	1640	1/1	0.85	-	49,49,49,49	0
57	MG	DA	9459	1/1	0.53	-	3,3,3,3	0
57	MG	DA	9591	1/1	0.23	-	52,52,52,52	0
57	MG	CA	1678	1/1	0.24	-	17,17,17,17	0
57	MG	CX	101	1/1	0.24	-	25,25,25,25	0
57	MG	BA	3120	1/1	0.66	-	24,24,24,24	0
57	MG	DA	9584	1/1	0.35	-	0,0,0,0	0
59	ZN	CN	101	1/1	0.18	-	171,171,171,171	0
57	MG	DA	9494	1/1	0.39	-	39,39,39,39	0
57	MG	BA	3205	1/1	0.51	-	0,0,0,0	0
57	MG	DA	9351	1/1	0.46	-	2,2,2,2	0
57	MG	BA	3266	1/1	0.42	-	33,33,33,33	0
57	MG	BA	3100	1/1	0.16	-	21,21,21,21	0
57	MG	DA	9598	1/1	0.44	-	14,14,14,14	0
57	MG	DA	9599	1/1	0.30	-	20,20,20,20	0
57	MG	BA	3163	1/1	0.32	-	28,28,28,28	0
57	MG	BA	3257	1/1	0.31	-	21,21,21,21	0
57	MG	DA	9660	1/1	0.27	-	176,176,176,176	0
57	MG	DA	9335	1/1	0.34	-	21,21,21,21	0
57	MG	BA	3118	1/1	0.58	-	28,28,28,28	0
57	MG	DA	9322	1/1	0.24	-	8,8,8,8	0
57	MG	AA	7082	1/1	0.28	-	24,24,24,24	0
57	MG	BA	3273	1/1	0.26	-	71,71,71,71	0
57	MG	DA	9366	1/1	0.47	-	1,1,1,1	0
57	MG	DA	9548	1/1	0.72	-	26,26,26,26	0
57	MG	BA	3119	1/1	0.33	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3225	1/1	0.29	-	2,2,2,2	0
57	MG	BA	3178	1/1	0.25	-	28,28,28,28	0
57	MG	DA	9449	1/1	0.41	-	0,0,0,0	0
57	MG	BA	3160	1/1	0.33	-	22,22,22,22	0
57	MG	CA	1691	1/1	0.69	-	91,91,91,91	0
57	MG	DA	9356	1/1	0.31	-	1,1,1,1	0
57	MG	CA	1607	1/1	0.53	-	32,32,32,32	0
57	MG	DA	9567	1/1	0.51	-	31,31,31,31	0
57	MG	BA	3184	1/1	0.98	-	22,22,22,22	0
57	MG	BA	3223	1/1	0.22	-	9,9,9,9	0
57	MG	DA	9588	1/1	0.13	-	16,16,16,16	0
57	MG	CA	1633	1/1	0.27	-	9,9,9,9	0
57	MG	CA	1704	1/1	0.96	-	28,28,28,28	0
57	MG	DA	9637	1/1	0.34	-	18,18,18,18	0
57	MG	DA	9457	1/1	0.62	-	13,13,13,13	0
57	MG	BA	3308	1/1	0.44	-	37,37,37,37	0
57	MG	BA	3148	1/1	0.36	-	16,16,16,16	0
57	MG	CA	1603	1/1	0.16	-	0,0,0,0	0
57	MG	DA	9615	1/1	0.70	-	45,45,45,45	0
57	MG	DA	9344	1/1	0.40	-	33,33,33,33	0
57	MG	CV	102	1/1	0.22	-	1,1,1,1	0
57	MG	BA	3075	1/1	0.70	-	12,12,12,12	0
57	MG	CA	1679	1/1	0.30	-	9,9,9,9	0
57	MG	DA	9667	1/1	0.36	-	10,10,10,10	0
57	MG	AA	7097	1/1	0.46	-	20,20,20,20	0
57	MG	BA	3151	1/1	0.13	-	12,12,12,12	0
57	MG	BA	3040	1/1	0.28	-	0,0,0,0	0
57	MG	DA	9425	1/1	0.44	-	37,37,37,37	0
57	MG	AA	7061	1/1	0.26	-	19,19,19,19	0
57	MG	CA	1723	1/1	0.34	-	15,15,15,15	0
57	MG	BA	3290	1/1	0.75	-	19,19,19,19	1
57	MG	BO	201	1/1	0.43	-	45,45,45,45	0
57	MG	D0	102	1/1	0.50	-	15,15,15,15	0
57	MG	BA	3070	1/1	0.42	-	34,34,34,34	0
57	MG	DA	9387	1/1	0.70	-	1,1,1,1	0
57	MG	CA	1673	1/1	0.26	-	18,18,18,18	0
57	MG	DA	9465	1/1	0.40	-	34,34,34,34	0
57	MG	BA	3288	1/1	0.13	-	18,18,18,18	0
57	MG	BA	3214	1/1	0.33	-	39,39,39,39	0
57	MG	DA	9655	1/1	0.93	-	35,35,35,35	0
57	MG	BA	3248	1/1	0.78	-	49,49,49,49	0
57	MG	BA	3171	1/1	0.44	-	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	7031	1/1	0.20	-	44,44,44,44	0
57	MG	BA	3134	1/1	0.49	-	21,21,21,21	0
57	MG	DA	9357	1/1	0.36	-	0,0,0,0	0
57	MG	DA	9478	1/1	0.40	-	13,13,13,13	0
57	MG	AA	7048	1/1	0.26	-	27,27,27,27	0
57	MG	BA	3299	1/1	0.49	-	10,10,10,10	0
57	MG	DA	9454	1/1	0.47	-	34,34,34,34	0
57	MG	CA	1717	1/1	0.32	-	11,11,11,11	0
57	MG	BA	3243	1/1	0.44	-	5,5,5,5	0
57	MG	BA	3285	1/1	1.75	-	32,32,32,32	1
57	MG	BA	3011	1/1	0.56	-	36,36,36,36	0
57	MG	DA	9492	1/1	0.11	-	76,76,76,76	0
57	MG	BA	3211	1/1	0.15	-	2,2,2,2	0
57	MG	BA	3274	1/1	0.25	-	8,8,8,8	1
57	MG	DA	9330	1/1	0.35	-	0,0,0,0	0
57	MG	DA	9618	1/1	0.80	-	28,28,28,28	1
57	MG	DA	9677	1/1	0.51	-	27,27,27,27	0
57	MG	AA	7054	1/1	1.00	-	29,29,29,29	0
57	MG	AA	7105	1/1	0.67	-	42,42,42,42	0
57	MG	DA	9520	1/1	0.47	-	2,2,2,2	0
57	MG	BB	203	1/1	0.65	-	16,16,16,16	1
57	MG	DA	9477	1/1	0.62	-	36,36,36,36	0
57	MG	DA	9409	1/1	0.31	-	4,4,4,4	0
57	MG	DA	9695	1/1	0.42	-	63,63,63,63	0
57	MG	BA	3032	1/1	0.22	-	18,18,18,18	0
57	MG	AA	7025	1/1	0.20	-	1,1,1,1	0
57	MG	DA	9315	1/1	0.10	-	26,26,26,26	0
57	MG	DA	9607	1/1	0.33	-	49,49,49,49	0
57	MG	DA	9305	1/1	0.44	-	0,0,0,0	0
57	MG	DA	9342	1/1	0.14	-	0,0,0,0	0
57	MG	AA	7107	1/1	0.44	-	24,24,24,24	0
57	MG	DA	9534	1/1	0.52	-	1,1,1,1	0
57	MG	BA	3199	1/1	0.47	-	1,1,1,1	0
57	MG	DA	9577	1/1	0.89	-	102,102,102,102	0
57	MG	DA	9521	1/1	0.57	-	2,2,2,2	0
58	PAR	CA	1741	42/42	0.31	-	55,55,55,55	0
57	MG	CA	1666	1/1	0.39	-	66,66,66,66	0
57	MG	AV	103	1/1	0.27	-	7,7,7,7	1
57	MG	CA	1621	1/1	0.39	-	52,52,52,52	0
57	MG	DB	202	1/1	0.21	-	28,28,28,28	0
57	MG	AA	7039	1/1	0.36	-	11,11,11,11	0
57	MG	DA	9350	1/1	0.19	-	48,48,48,48	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3043	1/1	0.22	-	8,8,8,8	0
57	MG	DA	9424	1/1	0.53	-	5,5,5,5	0
57	MG	BA	3302	1/1	0.51	-	8,8,8,8	0
57	MG	DA	9581	1/1	0.43	-	4,4,4,4	0
57	MG	CV	104	1/1	0.30	-	22,22,22,22	1
57	MG	DA	9507	1/1	0.53	-	2,2,2,2	0
57	MG	CA	1732	1/1	0.53	-	27,27,27,27	0
57	MG	BA	3124	1/1	0.20	-	17,17,17,17	0
57	MG	DA	9326	1/1	0.24	-	1,1,1,1	0
57	MG	BA	3181	1/1	0.48	-	1,1,1,1	0
57	MG	BA	3249	1/1	0.39	-	25,25,25,25	0
57	MG	DA	9587	1/1	0.27	-	2,2,2,2	0
57	MG	BA	3224	1/1	0.21	-	5,5,5,5	0
57	MG	DA	9616	1/1	0.58	-	54,54,54,54	0
57	MG	BA	3023	1/1	0.28	-	4,4,4,4	0
57	MG	DA	9501	1/1	0.48	-	42,42,42,42	0
57	MG	BA	3232	1/1	0.18	-	44,44,44,44	0
57	MG	BA	3303	1/1	0.33	-	19,19,19,19	0
57	MG	DA	9485	1/1	0.40	-	15,15,15,15	0
57	MG	BA	3155	1/1	0.57	-	33,33,33,33	0
57	MG	CA	1731	1/1	0.15	-	30,30,30,30	0
57	MG	BA	3056	1/1	0.25	-	5,5,5,5	0
57	MG	BA	3152	1/1	0.32	-	18,18,18,18	0
57	MG	DA	9654	1/1	0.34	-	15,15,15,15	0
57	MG	BA	3284	1/1	0.32	-	21,21,21,21	0
57	MG	DA	9590	1/1	0.46	-	1,1,1,1	0
57	MG	AA	7109	1/1	0.40	-	33,33,33,33	0
57	MG	BA	3220	1/1	0.73	-	56,56,56,56	0
57	MG	BA	3054	1/1	0.32	-	14,14,14,14	0
57	MG	DA	9518	1/1	0.35	-	0,0,0,0	0
57	MG	BA	3047	1/1	0.32	-	0,0,0,0	0
57	MG	CA	1675	1/1	0.40	-	55,55,55,55	0
57	MG	DA	9657	1/1	0.34	-	29,29,29,29	0
57	MG	BA	3007	1/1	0.63	-	4,4,4,4	0
57	MG	DA	9531	1/1	0.37	-	1,1,1,1	0
57	MG	BA	3182	1/1	0.57	-	2,2,2,2	0
57	MG	AA	7072	1/1	0.15	-	23,23,23,23	0
57	MG	DA	9571	1/1	0.47	-	0,0,0,0	0
57	MG	BA	3115	1/1	0.25	-	33,33,33,33	0
57	MG	CA	1602	1/1	0.17	-	14,14,14,14	0
57	MG	AA	7049	1/1	0.27	-	41,41,41,41	0
57	MG	BA	3014	1/1	0.28	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3216	1/1	0.49	-	48,48,48,48	0
57	MG	CA	1601	1/1	0.38	-	39,39,39,39	0
57	MG	BA	3272	1/1	0.37	-	10,10,10,10	0
57	MG	DA	9533	1/1	0.30	-	0,0,0,0	0
57	MG	DA	9430	1/1	0.38	-	0,0,0,0	0
57	MG	DA	9568	1/1	0.37	-	3,3,3,3	0
57	MG	BA	3147	1/1	0.68	-	48,48,48,48	0
57	MG	AA	7104	1/1	0.15	-	33,33,33,33	0
57	MG	CA	1631	1/1	0.89	-	22,22,22,22	0
57	MG	DA	9479	1/1	0.62	-	0,0,0,0	0
57	MG	DA	9604	1/1	0.31	-	21,21,21,21	0
57	MG	BA	3141	1/1	0.28	-	18,18,18,18	0
57	MG	CA	1612	1/1	0.30	-	31,31,31,31	0
57	MG	AA	7013	1/1	0.38	-	27,27,27,27	0
57	MG	CA	1647	1/1	0.35	-	6,6,6,6	0
57	MG	BA	3082	1/1	0.32	-	23,23,23,23	0
57	MG	BA	3162	1/1	0.75	-	4,4,4,4	0
57	MG	DA	9336	1/1	0.30	-	52,52,52,52	0
57	MG	DA	9569	1/1	0.85	-	54,54,54,54	0
57	MG	CV	105	1/1	0.21	-	69,69,69,69	0
57	MG	DA	9539	1/1	0.30	-	35,35,35,35	0
57	MG	BB	204	1/1	0.30	-	23,23,23,23	0
57	MG	CA	1668	1/1	0.35	-	56,56,56,56	0
57	MG	BA	3202	1/1	0.50	-	7,7,7,7	0
57	MG	DE	302	1/1	0.22	-	35,35,35,35	0
57	MG	CA	1610	1/1	0.64	-	58,58,58,58	0
57	MG	DA	9469	1/1	0.54	-	17,17,17,17	0
57	MG	DA	9487	1/1	0.26	-	71,71,71,71	0
57	MG	AA	7045	1/1	0.77	-	38,38,38,38	0
57	MG	AA	7065	1/1	0.38	-	23,23,23,23	0
57	MG	BA	3179	1/1	0.30	-	10,10,10,10	0
57	MG	CA	1642	1/1	0.36	-	54,54,54,54	0
57	MG	DA	9691	1/1	0.41	-	12,12,12,12	0
57	MG	DA	9648	1/1	0.32	-	34,34,34,34	0
57	MG	DA	9302	1/1	0.17	-	34,34,34,34	0
57	MG	DA	9375	1/1	0.53	-	0,0,0,0	0
57	MG	DA	9622	1/1	0.56	-	36,36,36,36	0
57	MG	AA	7084	1/1	0.13	-	49,49,49,49	0
57	MG	DA	9448	1/1	0.37	-	18,18,18,18	0
57	MG	CA	1645	1/1	0.35	-	20,20,20,20	0
57	MG	DA	9620	1/1	0.40	-	26,26,26,26	0
57	MG	DA	9511	1/1	0.80	-	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9378	1/1	0.33	-	29,29,29,29	0
57	MG	DA	9642	1/1	0.30	-	1,1,1,1	0
57	MG	BA	3038	1/1	0.15	-	31,31,31,31	0
57	MG	DA	9601	1/1	0.37	-	31,31,31,31	0
57	MG	BA	3076	1/1	0.24	-	18,18,18,18	0
57	MG	BA	3291	1/1	0.15	-	22,22,22,22	0
57	MG	DA	9389	1/1	0.14	-	11,11,11,11	0
57	MG	DA	9463	1/1	0.25	-	12,12,12,12	0
57	MG	DA	9493	1/1	0.27	-	1,1,1,1	0
57	MG	DA	9675	1/1	0.29	-	11,11,11,11	0
57	MG	AA	7004	1/1	0.29	-	30,30,30,30	0
57	MG	CA	1711	1/1	0.14	-	26,26,26,26	0
57	MG	DA	9406	1/1	0.16	-	32,32,32,32	0
57	MG	DA	9645	1/1	0.66	-	4,4,4,4	0
57	MG	CA	1648	1/1	0.45	-	23,23,23,23	0
57	MG	BA	3300	1/1	0.43	-	1,1,1,1	0
57	MG	DA	9500	1/1	0.22	-	1,1,1,1	0
57	MG	BA	3061	1/1	0.24	-	32,32,32,32	0
57	MG	AA	7083	1/1	0.54	-	18,18,18,18	0
57	MG	AA	7075	1/1	0.47	-	53,53,53,53	0
57	MG	BA	3268	1/1	0.33	-	13,13,13,13	1
57	MG	AA	7028	1/1	0.84	-	30,30,30,30	0
57	MG	DA	9367	1/1	0.40	-	35,35,35,35	0
57	MG	AA	7026	1/1	0.43	-	30,30,30,30	0
57	MG	BA	3241	1/1	0.47	-	4,4,4,4	0
57	MG	AA	7050	1/1	1.06	-	29,29,29,29	0
57	MG	BA	3052	1/1	0.50	-	40,40,40,40	0
57	MG	DA	9380	1/1	1.55	-	23,23,23,23	1
57	MG	BA	3192	1/1	0.38	-	2,2,2,2	0
57	MG	BA	3001	1/1	0.38	-	38,38,38,38	0
57	MG	BA	3123	1/1	0.19	-	14,14,14,14	0
57	MG	AA	7077	1/1	0.16	-	22,22,22,22	0
57	MG	BA	3136	1/1	0.46	-	46,46,46,46	1
58	PAR	AA	7111	42/42	0.26	-	58,58,58,58	0
57	MG	AA	7024	1/1	0.51	-	27,27,27,27	0
57	MG	BA	3113	1/1	0.77	-	49,49,49,49	0
57	MG	DA	9365	1/1	0.25	-	1,1,1,1	0
57	MG	DA	9646	1/1	0.21	-	31,31,31,31	0
57	MG	DA	9440	1/1	0.51	-	25,25,25,25	0
57	MG	BA	3210	1/1	0.76	-	11,11,11,11	0
57	MG	B7	101	1/1	0.35	-	13,13,13,13	0
57	MG	DA	9314	1/1	0.32	-	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	7095	1/1	0.08	-	17,17,17,17	0
57	MG	CA	1735	1/1	0.46	-	29,29,29,29	0
57	MG	DA	9423	1/1	0.21	-	1,1,1,1	0
57	MG	BA	3264	1/1	0.60	-	36,36,36,36	0
57	MG	DU	203	1/1	0.13	-	0,0,0,0	1
57	MG	AE	201	1/1	0.37	-	45,45,45,45	0
57	MG	DA	9550	1/1	0.43	-	55,55,55,55	0
57	MG	DA	9419	1/1	0.88	-	10,10,10,10	1
57	MG	BA	3122	1/1	0.31	-	13,13,13,13	0
57	MG	CA	1613	1/1	0.93	-	31,31,31,31	0
57	MG	DA	9468	1/1	0.69	-	2,2,2,2	1
57	MG	AA	7003	1/1	0.11	-	27,27,27,27	0
57	MG	BA	3259	1/1	0.31	-	18,18,18,18	0
57	MG	BA	3177	1/1	0.19	-	0,0,0,0	0
57	MG	BA	3107	1/1	0.48	-	36,36,36,36	0
57	MG	CA	1686	1/1	0.22	-	77,77,77,77	0
57	MG	BA	3137	1/1	0.62	-	1,1,1,1	1
57	MG	DA	9345	1/1	0.51	-	19,19,19,19	0
57	MG	DB	204	1/1	0.72	-	0,0,0,0	1
57	MG	CA	1737	1/1	0.62	-	28,28,28,28	0
57	MG	AA	7015	1/1	0.30	-	4,4,4,4	0
57	MG	DA	9503	1/1	0.36	-	66,66,66,66	0
57	MG	DA	9562	1/1	0.60	-	2,2,2,2	0
57	MG	BA	3080	1/1	0.56	-	0,0,0,0	0
57	MG	DA	9374	1/1	0.37	-	28,28,28,28	0
57	MG	AA	7012	1/1	0.77	-	12,12,12,12	0
57	MG	CA	1739	1/1	0.64	-	36,36,36,36	0
57	MG	DA	9561	1/1	0.29	-	10,10,10,10	0
57	MG	BA	3261	1/1	0.34	-	10,10,10,10	0
57	MG	DA	9662	1/1	0.52	-	2,2,2,2	0
57	MG	DW	201	1/1	0.46	-	27,27,27,27	0
57	MG	DA	9443	1/1	0.20	-	37,37,37,37	0
57	MG	BA	3006	1/1	0.35	-	38,38,38,38	0
57	MG	DA	9332	1/1	0.40	-	34,34,34,34	0
57	MG	CA	1700	1/1	0.32	-	20,20,20,20	0
57	MG	BA	3078	1/1	0.41	-	2,2,2,2	0
57	MG	AA	7046	1/1	0.42	-	35,35,35,35	0
57	MG	CA	1656	1/1	0.22	-	22,22,22,22	0
57	MG	DD	7101	1/1	0.47	-	3,3,3,3	0
57	MG	DA	9475	1/1	0.66	-	26,26,26,26	0
57	MG	DA	9596	1/1	0.17	-	27,27,27,27	0
57	MG	DA	9558	1/1	0.15	-	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1649	1/1	0.11	-	33,33,33,33	0
57	MG	DA	9694	1/1	0.83	-	25,25,25,25	0
57	MG	CY	101	1/1	0.56	-	33,33,33,33	0
57	MG	DA	9549	1/1	0.72	-	44,44,44,44	0
57	MG	BA	3017	1/1	0.58	-	22,22,22,22	0
57	MG	BA	3313	1/1	0.26	-	42,42,42,42	0
57	MG	DA	9355	1/1	0.66	-	0,0,0,0	0
57	MG	DA	9613	1/1	0.24	-	5,5,5,5	0
57	MG	BA	3037	1/1	0.28	-	83,83,83,83	0
57	MG	DA	9605	1/1	0.20	-	19,19,19,19	0
57	MG	DA	9611	1/1	0.46	-	8,8,8,8	0
57	MG	DA	9522	1/1	0.47	-	2,2,2,2	0
57	MG	BA	3079	1/1	0.38	-	29,29,29,29	1
57	MG	DA	9639	1/1	0.49	-	57,57,57,57	0
57	MG	DA	9455	1/1	0.44	-	0,0,0,0	0
57	MG	BA	3139	1/1	0.47	-	0,0,0,0	0
57	MG	DA	9578	1/1	0.47	-	44,44,44,44	0
57	MG	BA	3276	1/1	0.51	-	31,31,31,31	0
57	MG	AA	7038	1/1	0.62	-	10,10,10,10	0
57	MG	BA	3067	1/1	0.77	-	2,2,2,2	0
59	ZN	AD	301	1/1	0.31	-	41,41,41,41	0
57	MG	BA	3150	1/1	0.28	-	1,1,1,1	0
57	MG	BA	3247	1/1	0.84	-	55,55,55,55	0
57	MG	DA	9461	1/1	0.32	-	13,13,13,13	0
57	MG	BA	3207	1/1	0.37	-	1,1,1,1	0
57	MG	BA	3222	1/1	0.37	-	5,5,5,5	0
57	MG	BA	3236	1/1	0.53	-	17,17,17,17	0
57	MG	BA	3146	1/1	0.72	-	0,0,0,0	0
57	MG	DA	9580	1/1	0.46	-	0,0,0,0	0
57	MG	BA	3174	1/1	0.15	-	31,31,31,31	0
57	MG	BA	3235	1/1	0.39	-	25,25,25,25	0
57	MG	DA	9438	1/1	0.38	-	21,21,21,21	0
57	MG	CA	1718	1/1	0.28	-	27,27,27,27	0
57	MG	BA	3185	1/1	0.27	-	14,14,14,14	0
57	MG	DA	9502	1/1	0.41	-	3,3,3,3	0
57	MG	AA	7017	1/1	0.08	-	29,29,29,29	0
57	MG	DA	9546	1/1	0.35	-	2,2,2,2	0
57	MG	BA	3022	1/1	0.23	-	40,40,40,40	0
57	MG	DA	9682	1/1	0.36	-	20,20,20,20	0
57	MG	BA	3190	1/1	0.46	-	8,8,8,8	0
57	MG	DA	9368	1/1	0.20	-	1,1,1,1	0
57	MG	BE	303	1/1	0.15	-	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3121	1/1	0.62	-	1,1,1,1	0
57	MG	DA	9470	1/1	0.28	-	0,0,0,0	0
57	MG	DA	9483	1/1	0.47	-	0,0,0,0	0
57	MG	CA	1667	1/1	0.31	-	12,12,12,12	0
57	MG	AA	7088	1/1	0.18	-	60,60,60,60	0
57	MG	DA	9688	1/1	0.43	-	78,78,78,78	0
57	MG	CA	1692	1/1	0.35	-	28,28,28,28	0
57	MG	DA	9498	1/1	0.50	-	2,2,2,2	0
57	MG	AA	7009	1/1	0.27	-	18,18,18,18	0
57	MG	DA	9442	1/1	0.49	-	36,36,36,36	0
57	MG	CA	1615	1/1	0.29	-	0,0,0,0	0
57	MG	DA	9422	1/1	0.92	-	56,56,56,56	0
57	MG	AA	7036	1/1	0.37	-	42,42,42,42	0
57	MG	AA	7108	1/1	0.46	-	27,27,27,27	0
57	MG	CA	1634	1/1	0.29	-	43,43,43,43	0
57	MG	DA	9508	1/1	0.25	-	0,0,0,0	0
57	MG	CA	1609	1/1	0.44	-	30,30,30,30	0
57	MG	BA	3254	1/1	0.78	-	54,54,54,54	0
57	MG	AA	7103	1/1	0.49	-	13,13,13,13	0
57	MG	DA	9334	1/1	0.41	-	27,27,27,27	0
57	MG	DA	9418	1/1	0.28	-	61,61,61,61	0
57	MG	CA	1644	1/1	0.15	-	45,45,45,45	0
57	MG	BA	3044	1/1	0.55	-	18,18,18,18	0
57	MG	DA	9408	1/1	0.23	-	3,3,3,3	0
57	MG	BB	201	1/1	0.14	-	34,34,34,34	0
57	MG	DA	9348	1/1	0.76	-	47,47,47,47	0
57	MG	BA	3198	1/1	0.35	-	0,0,0,0	0
57	MG	AA	7008	1/1	0.86	-	35,35,35,35	0
57	MG	AA	7078	1/1	0.27	-	30,30,30,30	0
57	MG	DA	9482	1/1	0.21	-	12,12,12,12	0
57	MG	CA	1604	1/1	0.41	-	15,15,15,15	0
57	MG	BA	3183	1/1	0.65	-	56,56,56,56	0
57	MG	DA	9333	1/1	0.09	-	31,31,31,31	0
57	MG	DA	9663	1/1	0.61	-	7,7,7,7	0
57	MG	DA	9373	1/1	0.18	-	0,0,0,0	0
57	MG	D5	101	1/1	0.35	-	7,7,7,7	0
57	MG	BA	3057	1/1	0.51	-	2,2,2,2	0
57	MG	DA	9412	1/1	0.34	-	27,27,27,27	0
57	MG	DA	9384	1/1	0.28	-	16,16,16,16	0
57	MG	DA	9363	1/1	0.24	-	1,1,1,1	0
57	MG	BA	3315	1/1	0.43	-	84,84,84,84	0
59	ZN	AN	101	1/1	0.09	-	147,147,147,147	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	9327	1/1	0.19	-	20,20,20,20	0
57	MG	DA	9394	1/1	0.46	-	16,16,16,16	0
57	MG	DA	9450	1/1	0.55	-	2,2,2,2	1
57	MG	BA	3073	1/1	0.68	-	8,8,8,8	0
57	MG	DU	201	1/1	0.27	-	30,30,30,30	1
57	MG	DA	9410	1/1	0.27	-	4,4,4,4	0
57	MG	CA	1669	1/1	0.10	-	10,10,10,10	0
57	MG	BF	301	1/1	0.19	-	39,39,39,39	0
57	MG	DB	205	1/1	0.16	-	6,6,6,6	1
57	MG	BA	3033	1/1	0.19	-	6,6,6,6	0
57	MG	BA	3168	1/1	0.64	-	36,36,36,36	0
57	MG	BA	3294	1/1	0.54	-	15,15,15,15	1
57	MG	CA	1662	1/1	0.18	-	29,29,29,29	0
57	MG	AA	7101	1/1	0.62	-	22,22,22,22	0
57	MG	AA	7059	1/1	0.56	-	96,96,96,96	0
57	MG	DA	9544	1/1	0.42	-	10,10,10,10	0
57	MG	AA	7060	1/1	0.13	-	8,8,8,8	0
57	MG	AA	7047	1/1	0.35	-	41,41,41,41	0
57	MG	DA	9395	1/1	0.21	-	29,29,29,29	0
57	MG	DA	9632	1/1	0.47	-	12,12,12,12	1
57	MG	DA	9636	1/1	0.26	-	16,16,16,16	0
57	MG	CA	1727	1/1	0.33	-	27,27,27,27	0
57	MG	BA	3024	1/1	0.65	-	22,22,22,22	0
57	MG	DA	9490	1/1	0.24	-	39,39,39,39	0
57	MG	CA	1659	1/1	0.32	-	28,28,28,28	0
57	MG	BA	3304	1/1	0.44	-	13,13,13,13	0
57	MG	DA	9338	1/1	0.66	-	58,58,58,58	0
57	MG	DA	9647	1/1	0.59	-	1,1,1,1	0
57	MG	BA	3093	1/1	0.30	-	49,49,49,49	0
57	MG	BA	3099	1/1	0.25	-	30,30,30,30	0
57	MG	DX	101	1/1	0.33	-	6,6,6,6	0
57	MG	BA	3279	1/1	0.27	-	31,31,31,31	0
57	MG	BA	3265	1/1	0.55	-	43,43,43,43	0
57	MG	CA	1699	1/1	0.40	-	45,45,45,45	1
57	MG	AA	7081	1/1	0.44	-	44,44,44,44	0
57	MG	AA	7019	1/1	0.55	-	16,16,16,16	0
57	MG	CA	1623	1/1	0.28	-	19,19,19,19	0
57	MG	DA	9328	1/1	0.34	-	1,1,1,1	0
57	MG	DA	9628	1/1	0.27	-	35,35,35,35	1
57	MG	CA	1709	1/1	0.55	-	68,68,68,68	0
57	MG	DA	9530	1/1	0.83	-	41,41,41,41	0
57	MG	BA	3229	1/1	0.21	-	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BP	201	1/1	0.21	-	166,166,166,166	0
57	MG	DA	9527	1/1	0.38	-	1,1,1,1	0
57	MG	AV	105	1/1	0.34	-	54,54,54,54	0
57	MG	DA	9331	1/1	0.20	-	8,8,8,8	0
57	MG	CA	1605	1/1	0.22	-	32,32,32,32	0
57	MG	CA	1632	1/1	0.17	-	18,18,18,18	0
57	MG	AA	7055	1/1	0.44	-	29,29,29,29	0
57	MG	DA	9557	1/1	0.30	-	25,25,25,25	0
57	MG	AA	7010	1/1	0.26	-	30,30,30,30	0
57	MG	AA	7029	1/1	0.26	-	41,41,41,41	0
57	MG	DA	9614	1/1	0.26	-	12,12,12,12	0
57	MG	DA	9385	1/1	0.23	-	5,5,5,5	0
57	MG	DA	9445	1/1	0.44	-	22,22,22,22	0
57	MG	BA	3109	1/1	0.21	-	66,66,66,66	0
57	MG	DA	9317	1/1	0.24	-	18,18,18,18	0
57	MG	DA	9529	1/1	0.28	-	0,0,0,0	0
57	MG	CA	1722	1/1	0.37	-	27,27,27,27	0
57	MG	DA	9404	1/1	0.31	-	12,12,12,12	0
57	MG	DA	9488	1/1	0.56	-	0,0,0,0	0
57	MG	DA	9451	1/1	0.52	-	35,35,35,35	0
57	MG	BA	3175	1/1	0.29	-	4,4,4,4	0
57	MG	DA	9541	1/1	0.38	-	2,2,2,2	0
57	MG	BA	3176	1/1	0.34	-	0,0,0,0	0
57	MG	BA	3105	1/1	0.67	-	26,26,26,26	0
57	MG	DA	9472	1/1	0.37	-	16,16,16,16	0
57	MG	DF	301	1/1	0.14	-	20,20,20,20	0
57	MG	DA	9626	1/1	0.15	-	8,8,8,8	1
57	MG	DA	9382	1/1	0.45	-	0,0,0,0	0
57	MG	CA	1740	1/1	0.56	-	48,48,48,48	0
57	MG	DA	9564	1/1	0.56	-	17,17,17,17	0
57	MG	DA	9525	1/1	0.28	-	4,4,4,4	0
57	MG	BA	3015	1/1	0.20	-	3,3,3,3	0
57	MG	DA	9413	1/1	0.37	-	3,3,3,3	0
57	MG	BA	3065	1/1	0.66	-	2,2,2,2	0
57	MG	DA	9665	1/1	0.99	-	9,9,9,9	0
57	MG	CA	1724	1/1	0.44	-	5,5,5,5	0
57	MG	BA	3028	1/1	0.61	-	44,44,44,44	0
57	MG	DA	9575	1/1	0.11	-	35,35,35,35	0
57	MG	DA	9589	1/1	0.17	-	32,32,32,32	0
57	MG	CA	1688	1/1	0.16	-	16,16,16,16	0
57	MG	BA	3165	1/1	0.58	-	0,0,0,0	0
57	MG	BA	3130	1/1	0.20	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3096	1/1	0.42	-	12,12,12,12	0
57	MG	DA	9582	1/1	0.91	-	21,21,21,21	0
57	MG	CA	1664	1/1	0.45	-	24,24,24,24	0
57	MG	BA	3233	1/1	0.48	-	19,19,19,19	0
57	MG	BA	3317	1/1	0.71	-	21,21,21,21	0
57	MG	AA	7057	1/1	0.21	-	44,44,44,44	0
57	MG	BE	301	1/1	0.23	-	0,0,0,0	0
57	MG	DA	9504	1/1	0.14	-	27,27,27,27	0
57	MG	BA	3167	1/1	0.17	-	30,30,30,30	0
57	MG	DA	9638	1/1	0.25	-	8,8,8,8	1
57	MG	BA	3106	1/1	0.49	-	34,34,34,34	0
57	MG	CA	1696	1/1	0.35	-	49,49,49,49	0
57	MG	DA	9464	1/1	0.13	-	25,25,25,25	0
57	MG	BA	3135	1/1	0.49	-	43,43,43,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.